

Supplementary Material for manuscript:

Square planar Pt(II) ion as electron donor in pnictogen bonding interactions

Sergi Burguera, Rosa M. Gomila, Antonio Bauzá and Antonio Frontera*

Department of Chemistry, Universitat de les Illes Balears, Crta. de Valldemossa km 7.5, 07122 Palma, Spain

* Correspondence: toni.frontera@uib.es

Table of contents:

Figure S1 (MEP of Pt complex in RUVBIU)
NBO analyses

Page 2

Pages 3-47

1. MEP surface

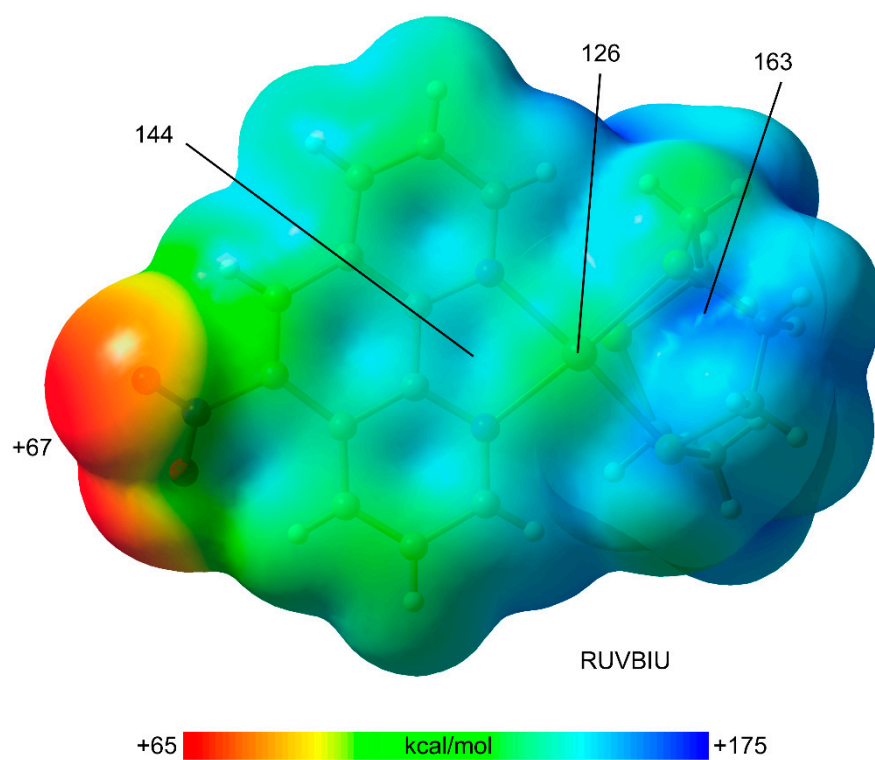
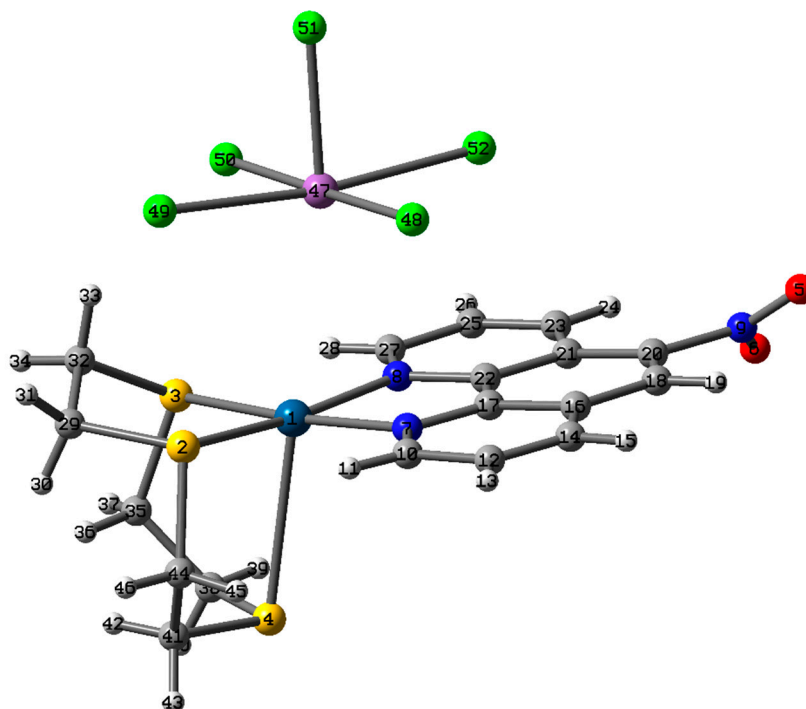


Figure S1. MEP surface of the cationic part of RUVBIU. The points at selected parts of the surface are given in kcal/mol

2. NBO second order analysis

2.1 RUVBIU



SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
=====				
from unit 1 to unit 2				
1. CR (1)Pt 1	414. RY (1) N 7	0.11	8.82	0.028
1. CR (1)Pt 1	440. RY (1) N 8	0.11	8.75	0.028
2. CR (2)Pt 1	440. RY (1) N 8	0.20	6.92	0.033
2. CR (2)Pt 1	441. RY (2) N 8	0.13	3.66	0.020
3. CR (3)Pt 1	414. RY (1) N 7	0.08	6.99	0.021
3. CR (3)Pt 1	440. RY (1) N 8	0.52	6.93	0.054
4. CR (4)Pt 1	414. RY (1) N 7	0.60	7.00	0.058
4. CR (4)Pt 1	415. RY (2) N 7	0.09	3.53	0.016
6. CR (2) S 2	440. RY (1) N 8	0.07	17.93	0.032
7. CR (3) S 2	440. RY (1) N 8	0.10	11.52	0.030
8. CR (4) S 2	440. RY (1) N 8	0.12	11.52	0.033
8. CR (4) S 2	441. RY (2) N 8	0.05	8.26	0.019
11. CR (2) S 3	414. RY (1) N 7	0.08	18.11	0.034
14. CR (5) S 3	414. RY (1) N 7	0.21	11.58	0.044
80. LP (1)Pt 1	195. BD* (1) N 7- C 10	0.25	0.76	0.012
80. LP (1)Pt 1	196. BD* (2) N 7- C 10	0.22	0.32	0.007
80. LP (1)Pt 1	197. BD* (1) N 7- C 17	0.36	0.73	0.014
80. LP (1)Pt 1	198. BD* (1) N 8- C 22	0.31	0.67	0.013
80. LP (1)Pt 1	199. BD* (1) N 8- C 27	0.16	0.81	0.010
80. LP (1)Pt 1	200. BD* (2) N 8- C 27	0.42	0.34	0.011
80. LP (1)Pt 1	203. BD* (1) C 10- C 12	0.19	0.82	0.011
80. LP (1)Pt 1	209. BD* (1) C 16- C 17	0.09	0.75	0.007
80. LP (1)Pt 1	216. BD* (1) C 21- C 22	0.16	0.81	0.010
80. LP (1)Pt 1	223. BD* (1) C 25- C 27	0.17	0.79	0.010
80. LP (1)Pt 1	414. RY (1) N 7	51.79	4.81	0.446
80. LP (1)Pt 1	415. RY (2) N 7	8.67	1.35	0.096
80. LP (1)Pt 1	416. RY (3) N 7	6.73	1.85	0.100
80. LP (1)Pt 1	417. RY (4) N 7	3.86	2.62	0.090
80. LP (1)Pt 1	420. RY (7) N 7	0.36	4.41	0.036
80. LP (1)Pt 1	422. RY (9) N 7	1.16	4.60	0.065
80. LP (1)Pt 1	423. RY (10) N 7	0.65	3.84	0.045
80. LP (1)Pt 1	424. RY (11) N 7	2.30	5.03	0.096
80. LP (1)Pt 1	425. RY (12) N 7	0.47	3.78	0.038
80. LP (1)Pt 1	426. RY (13) N 7	3.39	4.38	0.109
80. LP (1)Pt 1	427. RY (14) N 7	1.35	4.36	0.068
80. LP (1)Pt 1	428. RY (15) N 7	2.97	4.79	0.106
80. LP (1)Pt 1	429. RY (16) N 7	0.19	4.61	0.026
80. LP (1)Pt 1	430. RY (17) N 7	0.16	5.32	0.026
80. LP (1)Pt 1	431. RY (18) N 7	0.13	3.56	0.019
80. LP (1)Pt 1	432. RY (19) N 7	0.06	5.00	0.015
80. LP (1)Pt 1	433. RY (20) N 7	0.07	4.86	0.017
80. LP (1)Pt 1	434. RY (21) N 7	0.17	4.96	0.026
80. LP (1)Pt 1	435. RY (22) N 7	0.58	5.28	0.049
80. LP (1)Pt 1	436. RY (23) N 7	0.29	5.64	0.036
80. LP (1)Pt 1	437. RY (24) N 7	0.05	25.37	0.032
80. LP (1)Pt 1	439. RY (26) N 7	1.22	5.22	0.071
80. LP (1)Pt 1	440. RY (1) N 8	50.38	4.75	0.437

80. LP (1)Pt 1	441. RY (2) N 8	16.39	1.49	0.139
80. LP (1)Pt 1	442. RY (3) N 8	3.30	1.83	0.069
80. LP (1)Pt 1	443. RY (4) N 8	4.41	2.71	0.098
80. LP (1)Pt 1	444. RY (5) N 8	0.10	2.32	0.013
80. LP (1)Pt 1	445. RY (6) N 8	0.10	2.45	0.014
80. LP (1)Pt 1	446. RY (7) N 8	0.19	3.66	0.023
80. LP (1)Pt 1	447. RY (8) N 8	0.16	3.20	0.020
80. LP (1)Pt 1	448. RY (9) N 8	0.53	4.64	0.044
80. LP (1)Pt 1	449. RY (10) N 8	0.26	4.18	0.029
80. LP (1)Pt 1	450. RY (11) N 8	0.61	4.83	0.048
80. LP (1)Pt 1	451. RY (12) N 8	5.60	3.97	0.133
80. LP (1)Pt 1	452. RY (13) N 8	6.58	3.89	0.143
80. LP (1)Pt 1	453. RY (14) N 8	1.27	4.77	0.069
80. LP (1)Pt 1	454. RY (15) N 8	0.08	4.64	0.017
80. LP (1)Pt 1	456. RY (17) N 8	0.13	4.94	0.023
80. LP (1)Pt 1	460. RY (21) N 8	0.30	5.15	0.035
80. LP (1)Pt 1	461. RY (22) N 8	0.08	4.96	0.018
80. LP (1)Pt 1	462. RY (23) N 8	0.20	5.05	0.028
80. LP (1)Pt 1	464. RY (25) N 8	1.79	5.27	0.087
80. LP (1)Pt 1	465. RY (26) N 8	0.08	26.40	0.041
80. LP (1)Pt 1	492. RY (1) C 10	5.94	2.04	0.098
80. LP (1)Pt 1	493. RY (2) C 10	0.84	1.50	0.032
80. LP (1)Pt 1	494. RY (3) C 10	2.09	1.84	0.055
80. LP (1)Pt 1	495. RY (4) C 10	8.83	1.88	0.115
80. LP (1)Pt 1	496. RY (5) C 10	0.21	2.50	0.020
80. LP (1)Pt 1	497. RY (6) C 10	1.11	3.64	0.057
80. LP (1)Pt 1	498. RY (7) C 10	1.18	1.89	0.042
80. LP (1)Pt 1	499. RY (8) C 10	8.46	3.07	0.144
80. LP (1)Pt 1	500. RY (9) C 10	0.08	3.01	0.014
80. LP (1)Pt 1	501. RY (10) C 10	0.79	2.51	0.040
80. LP (1)Pt 1	502. RY (11) C 10	0.64	4.10	0.046
80. LP (1)Pt 1	504. RY (13) C 10	3.83	3.03	0.096
80. LP (1)Pt 1	505. RY (14) C 10	0.13	2.94	0.017
80. LP (1)Pt 1	507. RY (16) C 10	0.60	3.51	0.041
80. LP (1)Pt 1	508. RY (17) C 10	0.63	3.46	0.042
80. LP (1)Pt 1	509. RY (18) C 10	0.09	3.75	0.017
80. LP (1)Pt 1	518. RY (1) H 11	6.18	1.72	0.092
80. LP (1)Pt 1	519. RY (2) H 11	0.72	2.60	0.039
80. LP (1)Pt 1	521. RY (4) H 11	0.22	2.98	0.023
80. LP (1)Pt 1	522. RY (5) H 11	0.69	3.60	0.045
80. LP (1)Pt 1	524. RY (2) C 12	0.08	2.02	0.012
80. LP (1)Pt 1	526. RY (4) C 12	0.11	1.67	0.012
80. LP (1)Pt 1	529. RY (7) C 12	0.07	3.06	0.013
80. LP (1)Pt 1	531. RY (9) C 12	0.15	1.87	0.015
80. LP (1)Pt 1	532. RY (10) C 12	0.10	3.62	0.017
80. LP (1)Pt 1	533. RY (11) C 12	0.46	2.57	0.031
80. LP (1)Pt 1	534. RY (12) C 12	0.07	3.53	0.014
80. LP (1)Pt 1	537. RY (15) C 12	0.18	3.57	0.023
80. LP (1)Pt 1	539. RY (17) C 12	0.05	3.92	0.013
80. LP (1)Pt 1	556. RY (3) C 14	0.25	1.42	0.017
80. LP (1)Pt 1	557. RY (4) C 14	0.42	1.69	0.024
80. LP (1)Pt 1	560. RY (7) C 14	0.18	2.53	0.019
80. LP (1)Pt 1	562. RY (9) C 14	0.22	3.13	0.024
80. LP (1)Pt 1	564. RY (11) C 14	0.85	2.87	0.044
80. LP (1)Pt 1	565. RY (12) C 14	0.11	3.28	0.017
80. LP (1)Pt 1	566. RY (13) C 14	0.09	2.56	0.013
80. LP (1)Pt 1	569. RY (16) C 14	0.08	3.37	0.015
80. LP (1)Pt 1	581. RY (2) H 15	0.16	2.16	0.017
80. LP (1)Pt 1	585. RY (1) C 16	0.08	2.06	0.011
80. LP (1)Pt 1	586. RY (2) C 16	0.59	2.10	0.031
80. LP (1)Pt 1	587. RY (3) C 16	0.17	1.42	0.014
80. LP (1)Pt 1	588. RY (4) C 16	0.31	1.80	0.021
80. LP (1)Pt 1	590. RY (6) C 16	0.44	4.28	0.039
80. LP (1)Pt 1	592. RY (8) C 16	0.24	3.39	0.025
80. LP (1)Pt 1	593. RY (9) C 16	0.14	3.41	0.020
80. LP (1)Pt 1	596. RY (12) C 16	0.74	2.80	0.041
80. LP (1)Pt 1	597. RY (13) C 16	0.15	4.28	0.023
80. LP (1)Pt 1	598. RY (14) C 16	0.35	2.65	0.027
80. LP (1)Pt 1	601. RY (17) C 16	0.23	3.02	0.024
80. LP (1)Pt 1	611. RY (1) C 17	15.88	2.63	0.182
80. LP (1)Pt 1	612. RY (2) C 17	1.84	1.92	0.053
80. LP (1)Pt 1	613. RY (3) C 17	4.18	1.57	0.072
80. LP (1)Pt 1	614. RY (4) C 17	19.98	2.94	0.216
80. LP (1)Pt 1	615. RY (5) C 17	3.99	3.32	0.103
80. LP (1)Pt 1	616. RY (6) C 17	6.29	2.71	0.116
80. LP (1)Pt 1	617. RY (7) C 17	0.75	2.94	0.042
80. LP (1)Pt 1	619. RY (9) C 17	0.68	3.22	0.042
80. LP (1)Pt 1	620. RY (10) C 17	0.71	3.16	0.042
80. LP (1)Pt 1	621. RY (11) C 17	0.06	3.46	0.013
80. LP (1)Pt 1	622. RY (12) C 17	5.81	3.60	0.129
80. LP (1)Pt 1	623. RY (13) C 17	0.25	3.31	0.026
80. LP (1)Pt 1	624. RY (14) C 17	0.17	3.48	0.021
80. LP (1)Pt 1	625. RY (15) C 17	2.86	4.36	0.100
80. LP (1)Pt 1	626. RY (16) C 17	0.08	4.36	0.016
80. LP (1)Pt 1	628. RY (18) C 17	1.85	2.87	0.065
80. LP (1)Pt 1	629. RY (19) C 17	0.07	3.79	0.014
80. LP (1)Pt 1	630. RY (20) C 17	0.21	4.06	0.026
80. LP (1)Pt 1	631. RY (21) C 17	0.73	3.82	0.047
80. LP (1)Pt 1	632. RY (22) C 17	0.38	5.00	0.039
80. LP (1)Pt 1	633. RY (23) C 17	0.20	4.12	0.025
80. LP (1)Pt 1	636. RY (26) C 17	0.25	4.36	0.029
80. LP (1)Pt 1	648. RY (12) C 18	0.06	3.06	0.012
80. LP (1)Pt 1	663. RY (1) H 19	0.06	1.92	0.010
80. LP (1)Pt 1	671. RY (4) C 20	0.06	1.69	0.009
80. LP (1)Pt 1	675. RY (8) C 20	0.07	3.21	0.013
80. LP (1)Pt 1	694. RY (1) C 21	0.13	1.97	0.014
80. LP (1)Pt 1	695. RY (2) C 21	0.57	1.99	0.030
80. LP (1)Pt 1	696. RY (3) C 21	0.32	1.71	0.021
80. LP (1)Pt 1	697. RY (4) C 21	0.24	1.52	0.017
80. LP (1)Pt 1	699. RY (6) C 21	0.58	3.97	0.043
80. LP (1)Pt 1	704. RY (11) C 21	1.55	2.86	0.059
80. LP (1)Pt 1	706. RY (13) C 21	0.20	2.97	0.022
80. LP (1)Pt 1	707. RY (14) C 21	0.11	3.79	0.018

80.	LP	(1)	Pt	1	720.	RY	(1)	C	22	13.24	2.47	0.162
80.	LP	(1)	Pt	1	721.	RY	(2)	C	22	5.61	2.03	0.095
80.	LP	(1)	Pt	1	722.	RY	(3)	C	22	7.36	1.70	0.100
80.	LP	(1)	Pt	1	723.	RY	(4)	C	22	19.22	2.83	0.208
80.	LP	(1)	Pt	1	724.	RY	(5)	C	22	2.29	2.82	0.072
80.	LP	(1)	Pt	1	726.	RY	(7)	C	22	3.92	2.73	0.092
80.	LP	(1)	Pt	1	727.	RY	(8)	C	22	0.07	3.13	0.013
80.	LP	(1)	Pt	1	729.	RY	(10)	C	22	0.26	3.40	0.027
80.	LP	(1)	Pt	1	730.	RY	(11)	C	22	8.64	3.87	0.163
80.	LP	(1)	Pt	1	731.	RY	(12)	C	22	2.04	3.55	0.076
80.	LP	(1)	Pt	1	732.	RY	(13)	C	22	1.59	3.37	0.065
80.	LP	(1)	Pt	1	734.	RY	(15)	C	22	2.02	4.70	0.087
80.	LP	(1)	Pt	1	735.	RY	(16)	C	22	0.90	4.31	0.056
80.	LP	(1)	Pt	1	737.	RY	(18)	C	22	0.58	3.72	0.041
80.	LP	(1)	Pt	1	738.	RY	(19)	C	22	0.27	4.61	0.031
80.	LP	(1)	Pt	1	740.	RY	(21)	C	22	0.92	4.23	0.056
80.	LP	(1)	Pt	1	741.	RY	(22)	C	22	0.06	4.91	0.015
80.	LP	(1)	Pt	1	742.	RY	(23)	C	22	0.05	4.61	0.014
80.	LP	(1)	Pt	1	743.	RY	(24)	C	22	0.12	4.45	0.021
80.	LP	(1)	Pt	1	748.	RY	(3)	C	23	0.13	1.39	0.012
80.	LP	(1)	Pt	1	749.	RY	(4)	C	23	0.60	1.87	0.030
80.	LP	(1)	Pt	1	753.	RY	(8)	C	23	0.33	2.97	0.028
80.	LP	(1)	Pt	1	754.	RY	(9)	C	23	0.07	3.79	0.014
80.	LP	(1)	Pt	1	755.	RY	(10)	C	23	0.24	2.62	0.022
80.	LP	(1)	Pt	1	756.	RY	(11)	C	23	0.30	2.83	0.026
80.	LP	(1)	Pt	1	757.	RY	(12)	C	23	0.16	3.05	0.020
80.	LP	(1)	Pt	1	758.	RY	(13)	C	23	0.25	3.52	0.026
80.	LP	(1)	Pt	1	759.	RY	(14)	C	23	0.29	2.72	0.025
80.	LP	(1)	Pt	1	761.	RY	(16)	C	23	0.06	3.65	0.013
80.	LP	(1)	Pt	1	762.	RY	(17)	C	23	0.22	2.53	0.021
80.	LP	(1)	Pt	1	773.	RY	(2)	H	24	0.22	1.98	0.019
80.	LP	(1)	Pt	1	780.	RY	(4)	C	25	0.18	1.79	0.016
80.	LP	(1)	Pt	1	783.	RY	(7)	C	25	0.19	3.58	0.023
80.	LP	(1)	Pt	1	786.	RY	(10)	C	25	0.80	2.68	0.041
80.	LP	(1)	Pt	1	787.	RY	(11)	C	25	0.16	2.54	0.018
80.	LP	(1)	Pt	1	790.	RY	(14)	C	25	0.08	2.72	0.013
80.	LP	(1)	Pt	1	808.	RY	(1)	C	27	8.76	2.28	0.126
80.	LP	(1)	Pt	1	809.	RY	(2)	C	27	0.19	1.44	0.015
80.	LP	(1)	Pt	1	810.	RY	(3)	C	27	1.90	1.81	0.052
80.	LP	(1)	Pt	1	811.	RY	(4)	C	27	8.64	2.05	0.119
80.	LP	(1)	Pt	1	812.	RY	(5)	C	27	0.30	2.52	0.025
80.	LP	(1)	Pt	1	813.	RY	(6)	C	27	4.38	2.41	0.092
80.	LP	(1)	Pt	1	814.	RY	(7)	C	27	0.14	2.60	0.017
80.	LP	(1)	Pt	1	815.	RY	(8)	C	27	6.43	3.48	0.133
80.	LP	(1)	Pt	1	816.	RY	(9)	C	27	2.80	2.90	0.080
80.	LP	(1)	Pt	1	817.	RY	(10)	C	27	1.72	2.80	0.062
80.	LP	(1)	Pt	1	818.	RY	(11)	C	27	1.19	2.82	0.052
80.	LP	(1)	Pt	1	819.	RY	(12)	C	27	0.47	3.60	0.037
80.	LP	(1)	Pt	1	820.	RY	(13)	C	27	0.10	2.90	0.015
80.	LP	(1)	Pt	1	821.	RY	(14)	C	27	0.09	3.49	0.016
80.	LP	(1)	Pt	1	822.	RY	(15)	C	27	0.05	3.03	0.011
80.	LP	(1)	Pt	1	823.	RY	(16)	C	27	2.55	2.96	0.078
80.	LP	(1)	Pt	1	824.	RY	(17)	C	27	0.29	4.03	0.030
80.	LP	(1)	Pt	1	825.	RY	(18)	C	27	0.20	3.82	0.025
80.	LP	(1)	Pt	1	834.	RY	(1)	H	28	15.45	2.00	0.157
80.	LP	(1)	Pt	1	835.	RY	(2)	H	28	1.29	2.71	0.053
80.	LP	(1)	Pt	1	837.	RY	(4)	H	28	0.21	3.02	0.022
80.	LP	(1)	Pt	1	838.	RY	(5)	H	28	1.03	3.69	0.055
81.	LP	(2)	Pt	1	181.	LV	(1)	C	17	0.08	0.32	0.005
81.	LP	(2)	Pt	1	196.	BD*	(2)	N	7- C 10	0.38	0.38	0.011
81.	LP	(2)	Pt	1	200.	BD*	(2)	N	8- C 27	0.63	0.40	0.014
81.	LP	(2)	Pt	1	414.	RY	(1)	N	7	0.07	4.87	0.016
81.	LP	(2)	Pt	1	415.	RY	(2)	N	7	2.79	1.41	0.056
81.	LP	(2)	Pt	1	416.	RY	(3)	N	7	0.16	1.91	0.015
81.	LP	(2)	Pt	1	426.	RY	(13)	N	7	0.06	4.44	0.014
81.	LP	(2)	Pt	1	440.	RY	(1)	N	8	0.55	4.81	0.046
81.	LP	(2)	Pt	1	441.	RY	(2)	N	8	2.72	1.54	0.058
81.	LP	(2)	Pt	1	442.	RY	(3)	N	8	0.08	1.89	0.011
81.	LP	(2)	Pt	1	445.	RY	(6)	N	8	0.07	2.51	0.012
81.	LP	(2)	Pt	1	611.	RY	(1)	C	17	0.08	2.69	0.013
81.	LP	(2)	Pt	1	613.	RY	(3)	C	17	0.23	1.63	0.017
81.	LP	(2)	Pt	1	723.	RY	(4)	C	22	0.14	2.89	0.018
81.	LP	(2)	Pt	1	815.	RY	(8)	C	27	0.05	3.54	0.012
81.	LP	(2)	Pt	1	820.	RY	(13)	C	27	0.05	2.96	0.011
81.	LP	(2)	Pt	1	834.	RY	(1)	H	28	0.07	2.06	0.010
82.	LP	(3)	Pt	1	195.	BD*	(1)	N	7- C 10	0.48	0.84	0.018
82.	LP	(3)	Pt	1	197.	BD*	(1)	N	7- C 17	0.39	0.82	0.016
82.	LP	(3)	Pt	1	198.	BD*	(1)	N	8- C 22	0.44	0.75	0.016
82.	LP	(3)	Pt	1	199.	BD*	(1)	N	8- C 27	0.50	0.89	0.019
82.	LP	(3)	Pt	1	414.	RY	(1)	N	7	3.14	4.90	0.111
82.	LP	(3)	Pt	1	415.	RY	(2)	N	7	0.21	1.43	0.016
82.	LP	(3)	Pt	1	416.	RY	(3)	N	7	3.49	1.94	0.073
82.	LP	(3)	Pt	1	417.	RY	(4)	N	7	0.50	2.71	0.033
82.	LP	(3)	Pt	1	424.	RY	(11)	N	7	0.08	5.11	0.018
82.	LP	(3)	Pt	1	425.	RY	(12)	N	7	0.08	3.87	0.016
82.	LP	(3)	Pt	1	426.	RY	(13)	N	7	0.12	4.47	0.020
82.	LP	(3)	Pt	1	427.	RY	(14)	N	7	0.11	4.44	0.019
82.	LP	(3)	Pt	1	428.	RY	(15)	N	7	0.16	4.87	0.025
82.	LP	(3)	Pt	1	439.	RY	(26)	N	7	0.10	5.30	0.020
82.	LP	(3)	Pt	1	440.	RY	(1)	N	8	2.91	4.84	0.106
82.	LP	(3)	Pt	1	441.	RY	(2)	N	8	0.18	1.57	0.015
82.	LP	(3)	Pt	1	442.	RY	(3)	N	8	4.49	1.92	0.083
82.	LP	(3)	Pt	1	443.	RY	(4)	N	8	0.73	2.80	0.040
82.	LP	(3)	Pt	1	451.	RY	(12)	N	8	0.31	4.06	0.032
82.	LP	(3)	Pt	1	452.	RY	(13)	N	8	0.33	3.97	0.032
82.	LP	(3)	Pt	1	464.	RY	(25)	N	8	0.10	5.36	0.021
82.	LP	(3)	Pt	1	492.	RY	(1)	C	10	0.56	2.12	0.031
82.	LP	(3)	Pt	1	493.	RY	(2)	C	10	0.09	1.59	0.011
82.	LP	(3)	Pt	1	494.	RY	(3)	C	10	0.53	1.92	0.029
82.	LP	(3)	Pt	1	495.	RY	(4)	C	10	0.84	1.96	0.036
82.	LP	(3)	Pt	1	497.	RY	(6)	C	10	0.06	3.72	0.013
82.	LP	(3)	Pt	1	499.	RY	(8)	C	10	0.21	3.16	0.023
82.	LP	(3)	Pt	1	504.	RY	(13)	C	10	0.35	3.11	0.030

82. LP (3)Pt 1	507. RY (16) C 10	0.06	3.59	0.013
82. LP (3)Pt 1	518. RY (1) H 11	0.50	1.80	0.027
82. LP (3)Pt 1	519. RY (2) H 11	0.06	2.69	0.011
82. LP (3)Pt 1	611. RY (1) C 17	0.55	2.72	0.034
82. LP (3)Pt 1	612. RY (2) C 17	0.17	2.01	0.016
82. LP (3)Pt 1	613. RY (3) C 17	0.20	1.66	0.016
82. LP (3)Pt 1	614. RY (4) C 17	0.69	3.02	0.041
82. LP (3)Pt 1	615. RY (5) C 17	0.50	3.40	0.037
82. LP (3)Pt 1	616. RY (6) C 17	0.65	2.79	0.038
82. LP (3)Pt 1	619. RY (9) C 17	0.17	3.30	0.021
82. LP (3)Pt 1	622. RY (12) C 17	0.46	3.68	0.037
82. LP (3)Pt 1	623. RY (13) C 17	0.06	3.40	0.013
82. LP (3)Pt 1	625. RY (15) C 17	0.16	4.45	0.024
82. LP (3)Pt 1	628. RY (18) C 17	0.06	2.96	0.012
82. LP (3)Pt 1	699. RY (6) C 21	0.07	4.06	0.015
82. LP (3)Pt 1	720. RY (1) C 22	0.42	2.56	0.029
82. LP (3)Pt 1	721. RY (2) C 22	0.44	2.12	0.027
82. LP (3)Pt 1	722. RY (3) C 22	0.32	1.79	0.021
82. LP (3)Pt 1	723. RY (4) C 22	0.73	2.91	0.041
82. LP (3)Pt 1	724. RY (5) C 22	0.32	2.90	0.027
82. LP (3)Pt 1	726. RY (7) C 22	0.42	2.82	0.031
82. LP (3)Pt 1	730. RY (11) C 22	0.64	3.96	0.045
82. LP (3)Pt 1	731. RY (12) C 22	0.24	3.64	0.027
82. LP (3)Pt 1	732. RY (13) C 22	0.21	3.46	0.024
82. LP (3)Pt 1	734. RY (15) C 22	0.10	4.79	0.019
82. LP (3)Pt 1	735. RY (16) C 22	0.06	4.40	0.015
82. LP (3)Pt 1	808. RY (1) C 27	0.84	2.36	0.040
82. LP (3)Pt 1	810. RY (3) C 27	0.52	1.90	0.028
82. LP (3)Pt 1	811. RY (4) C 27	0.89	2.14	0.039
82. LP (3)Pt 1	813. RY (6) C 27	0.09	2.50	0.013
82. LP (3)Pt 1	815. RY (8) C 27	0.19	3.56	0.023
82. LP (3)Pt 1	816. RY (9) C 27	0.28	2.98	0.026
82. LP (3)Pt 1	817. RY (10) C 27	0.10	2.89	0.015
82. LP (3)Pt 1	818. RY (11) C 27	0.10	2.91	0.016
82. LP (3)Pt 1	823. RY (16) C 27	0.15	3.04	0.019
82. LP (3)Pt 1	834. RY (1) H 28	1.10	2.09	0.043
82. LP (3)Pt 1	835. RY (2) H 28	0.09	2.79	0.014
83. LP (4)Pt 1	195. BD* (1) N 7- C 10	0.11	0.82	0.008
83. LP (4)Pt 1	196. BD* (2) N 7- C 10	0.77	0.38	0.015
83. LP (4)Pt 1	197. BD* (1) N 7- C 17	0.11	0.79	0.008
83. LP (4)Pt 1	198. BD* (1) N 8- C 22	0.11	0.73	0.008
83. LP (4)Pt 1	199. BD* (1) N 8- C 27	0.09	0.87	0.008
83. LP (4)Pt 1	200. BD* (2) N 8- C 27	0.48	0.40	0.012
83. LP (4)Pt 1	414. RY (1) N 7	3.03	4.88	0.109
83. LP (4)Pt 1	415. RY (2) N 7	2.04	1.41	0.048
83. LP (4)Pt 1	416. RY (3) N 7	1.32	1.92	0.045
83. LP (4)Pt 1	417. RY (4) N 7	0.11	2.69	0.016
83. LP (4)Pt 1	422. RY (9) N 7	0.07	4.67	0.016
83. LP (4)Pt 1	424. RY (11) N 7	0.15	5.09	0.025
83. LP (4)Pt 1	427. RY (14) N 7	0.21	4.42	0.027
83. LP (4)Pt 1	428. RY (15) N 7	0.14	4.85	0.024
83. LP (4)Pt 1	440. RY (1) N 8	3.29	4.81	0.112
83. LP (4)Pt 1	441. RY (2) N 8	0.47	1.55	0.024
83. LP (4)Pt 1	442. RY (3) N 8	1.15	1.90	0.042
83. LP (4)Pt 1	443. RY (4) N 8	0.13	2.78	0.017
83. LP (4)Pt 1	451. RY (12) N 8	0.29	4.04	0.031
83. LP (4)Pt 1	452. RY (13) N 8	0.29	3.95	0.030
83. LP (4)Pt 1	454. RY (15) N 8	0.06	4.70	0.015
83. LP (4)Pt 1	464. RY (25) N 8	0.06	5.34	0.016
83. LP (4)Pt 1	492. RY (1) C 10	0.14	2.10	0.016
83. LP (4)Pt 1	493. RY (2) C 10	0.13	1.56	0.013
83. LP (4)Pt 1	495. RY (4) C 10	0.36	1.94	0.024
83. LP (4)Pt 1	497. RY (6) C 10	0.07	3.70	0.014
83. LP (4)Pt 1	499. RY (8) C 10	0.52	3.14	0.036
83. LP (4)Pt 1	501. RY (10) C 10	0.06	2.57	0.011
83. LP (4)Pt 1	504. RY (13) C 10	0.23	3.09	0.024
83. LP (4)Pt 1	518. RY (1) H 11	0.20	1.78	0.017
83. LP (4)Pt 1	611. RY (1) C 17	0.89	2.70	0.044
83. LP (4)Pt 1	613. RY (3) C 17	0.43	1.63	0.024
83. LP (4)Pt 1	614. RY (4) C 17	0.94	3.00	0.047
83. LP (4)Pt 1	615. RY (5) C 17	0.11	3.38	0.017
83. LP (4)Pt 1	616. RY (6) C 17	0.21	2.77	0.021
83. LP (4)Pt 1	620. RY (10) C 17	0.07	3.23	0.014
83. LP (4)Pt 1	622. RY (12) C 17	0.28	3.66	0.029
83. LP (4)Pt 1	625. RY (15) C 17	0.13	4.43	0.022
83. LP (4)Pt 1	628. RY (18) C 17	0.06	2.93	0.012
83. LP (4)Pt 1	704. RY (11) C 21	0.08	2.92	0.014
83. LP (4)Pt 1	720. RY (1) C 22	0.84	2.54	0.041
83. LP (4)Pt 1	721. RY (2) C 22	0.16	2.10	0.016
83. LP (4)Pt 1	722. RY (3) C 22	0.79	1.77	0.033
83. LP (4)Pt 1	723. RY (4) C 22	0.70	2.89	0.040
83. LP (4)Pt 1	724. RY (5) C 22	0.07	2.88	0.013
83. LP (4)Pt 1	726. RY (7) C 22	0.11	2.79	0.015
83. LP (4)Pt 1	730. RY (11) C 22	0.30	3.94	0.031
83. LP (4)Pt 1	731. RY (12) C 22	0.17	3.61	0.022
83. LP (4)Pt 1	734. RY (15) C 22	0.10	4.76	0.020
83. LP (4)Pt 1	808. RY (1) C 27	0.25	2.34	0.022
83. LP (4)Pt 1	809. RY (2) C 27	0.10	1.51	0.011
83. LP (4)Pt 1	811. RY (4) C 27	0.39	2.12	0.026
83. LP (4)Pt 1	813. RY (6) C 27	0.17	2.48	0.019
83. LP (4)Pt 1	815. RY (8) C 27	0.44	3.54	0.035
83. LP (4)Pt 1	816. RY (9) C 27	0.13	2.96	0.018
83. LP (4)Pt 1	817. RY (10) C 27	0.07	2.86	0.013
83. LP (4)Pt 1	818. RY (11) C 27	0.07	2.88	0.012
83. LP (4)Pt 1	823. RY (16) C 27	0.08	3.02	0.014
83. LP (4)Pt 1	834. RY (1) H 28	0.60	2.07	0.031
83. LP (4)Pt 1	835. RY (2) H 28	0.06	2.77	0.011
83. LP (4)Pt 1	838. RY (5) H 28	0.05	3.76	0.013
84. LP (1) S 2	414. RY (1) N 7	0.56	4.91	0.047
84. LP (1) S 2	415. RY (2) N 7	0.11	1.45	0.011
84. LP (1) S 2	424. RY (11) N 7	0.05	5.13	0.015
84. LP (1) S 2	426. RY (13) N 7	0.07	4.48	0.015
84. LP (1) S 2	428. RY (15) N 7	0.06	4.89	0.015

84. LP (1) S 2	440. RY (1) N 8	0.25	4.85	0.031
84. LP (1) S 2	441. RY (2) N 8	0.05	1.59	0.008
84. LP (1) S 2	443. RY (4) N 8	0.13	2.81	0.017
84. LP (1) S 2	452. RY (13) N 8	0.07	3.99	0.015
84. LP (1) S 2	495. RY (4) C 10	0.12	1.98	0.014
84. LP (1) S 2	499. RY (8) C 10	0.24	3.17	0.024
84. LP (1) S 2	504. RY (13) C 10	0.08	3.13	0.015
84. LP (1) S 2	518. RY (1) H 11	0.15	1.82	0.015
84. LP (1) S 2	611. RY (1) C 17	0.23	2.73	0.022
84. LP (1) S 2	614. RY (4) C 17	0.21	3.04	0.022
84. LP (1) S 2	615. RY (5) C 17	0.06	3.42	0.013
84. LP (1) S 2	616. RY (6) C 17	0.11	2.81	0.016
84. LP (1) S 2	622. RY (12) C 17	0.07	3.70	0.014
84. LP (1) S 2	720. RY (1) C 22	0.12	2.57	0.016
84. LP (1) S 2	722. RY (3) C 22	0.10	1.80	0.012
84. LP (1) S 2	723. RY (4) C 22	0.28	2.93	0.025
84. LP (1) S 2	724. RY (5) C 22	0.06	2.92	0.012
84. LP (1) S 2	726. RY (7) C 22	0.08	2.83	0.013
84. LP (1) S 2	730. RY (11) C 22	0.13	3.97	0.021
84. LP (1) S 2	808. RY (1) C 27	0.09	2.38	0.013
84. LP (1) S 2	811. RY (4) C 27	0.10	2.15	0.013
84. LP (1) S 2	815. RY (8) C 27	0.07	3.58	0.014
84. LP (1) S 2	834. RY (1) H 28	0.19	2.11	0.018
85. LP (1) S 3	223. BD* (1) C 25- C 27	0.07	0.88	0.007
85. LP (1) S 3	224. BD* (1) C 27- H 28	0.07	1.11	0.008
85. LP (1) S 3	417. RY (4) N 7	0.05	2.72	0.011
85. LP (1) S 3	440. RY (1) N 8	0.18	4.85	0.026
85. LP (1) S 3	441. RY (2) N 8	0.05	1.58	0.008
85. LP (1) S 3	452. RY (13) N 8	0.06	3.98	0.013
85. LP (1) S 3	614. RY (4) C 17	0.10	3.04	0.015
85. LP (1) S 3	720. RY (1) C 22	0.07	2.57	0.012
85. LP (1) S 3	723. RY (4) C 22	0.06	2.92	0.012
85. LP (1) S 3	811. RY (4) C 27	0.06	2.15	0.010
85. LP (1) S 3	813. RY (6) C 27	0.05	2.51	0.010
85. LP (1) S 3	815. RY (8) C 27	0.14	3.57	0.020
85. LP (1) S 3	817. RY (10) C 27	0.08	2.90	0.013
85. LP (1) S 3	834. RY (1) H 28	0.19	2.10	0.018
86. LP (1) S 4	414. RY (1) N 7	0.23	4.96	0.030
86. LP (1) S 4	440. RY (1) N 8	0.21	4.89	0.029
86. LP (1) S 4	499. RY (8) C 10	0.06	3.21	0.012
86. LP (1) S 4	611. RY (1) C 17	0.09	2.77	0.014
86. LP (1) S 4	614. RY (4) C 17	0.11	3.08	0.016
86. LP (1) S 4	720. RY (1) C 22	0.07	2.61	0.012
86. LP (1) S 4	722. RY (3) C 22	0.05	1.84	0.009
86. LP (1) S 4	723. RY (4) C 22	0.11	2.97	0.016
86. LP (1) S 4	730. RY (11) C 22	0.06	4.01	0.013
86. LP (1) S 4	808. RY (1) C 27	0.06	2.42	0.010
86. LP (1) S 4	811. RY (4) C 27	0.06	2.20	0.010
86. LP (1) S 4	834. RY (1) H 28	0.09	2.15	0.012
87. LP (2) S 4	196. BD* (2) N 7- C 10	0.10	0.18	0.004
87. LP (2) S 4	197. BD* (1) N 7- C 17	0.08	0.59	0.006
87. LP (2) S 4	200. BD* (2) N 8- C 27	0.14	0.19	0.005
87. LP (2) S 4	414. RY (1) N 7	4.11	4.67	0.124
87. LP (2) S 4	415. RY (2) N 7	0.47	1.20	0.021
87. LP (2) S 4	416. RY (3) N 7	0.41	1.71	0.024
87. LP (2) S 4	417. RY (4) N 7	0.57	2.48	0.034
87. LP (2) S 4	422. RY (9) N 7	0.20	4.46	0.027
87. LP (2) S 4	423. RY (10) N 7	0.07	3.69	0.014
87. LP (2) S 4	424. RY (11) N 7	0.23	4.88	0.030
87. LP (2) S 4	426. RY (13) N 7	0.42	4.24	0.038
87. LP (2) S 4	427. RY (14) N 7	0.18	4.22	0.025
87. LP (2) S 4	428. RY (15) N 7	0.32	4.64	0.034
87. LP (2) S 4	439. RY (26) N 7	0.09	5.08	0.019
87. LP (2) S 4	440. RY (1) N 8	4.10	4.61	0.123
87. LP (2) S 4	441. RY (2) N 8	0.96	1.34	0.032
87. LP (2) S 4	442. RY (3) N 8	0.19	1.69	0.016
87. LP (2) S 4	443. RY (4) N 8	0.62	2.57	0.036
87. LP (2) S 4	448. RY (9) N 8	0.11	4.50	0.020
87. LP (2) S 4	450. RY (11) N 8	0.05	4.69	0.014
87. LP (2) S 4	451. RY (12) N 8	0.62	3.83	0.044
87. LP (2) S 4	452. RY (13) N 8	0.82	3.74	0.049
87. LP (2) S 4	453. RY (14) N 8	0.13	4.63	0.022
87. LP (2) S 4	464. RY (25) N 8	0.12	5.13	0.022
87. LP (2) S 4	492. RY (1) C 10	0.64	1.90	0.031
87. LP (2) S 4	493. RY (2) C 10	0.08	1.36	0.009
87. LP (2) S 4	494. RY (3) C 10	0.20	1.70	0.017
87. LP (2) S 4	495. RY (4) C 10	0.95	1.74	0.036
87. LP (2) S 4	497. RY (6) C 10	0.10	3.49	0.017
87. LP (2) S 4	498. RY (7) C 10	0.09	1.75	0.011
87. LP (2) S 4	499. RY (8) C 10	0.89	2.93	0.046
87. LP (2) S 4	501. RY (10) C 10	0.10	2.37	0.014
87. LP (2) S 4	502. RY (11) C 10	0.07	3.96	0.015
87. LP (2) S 4	504. RY (13) C 10	0.48	2.88	0.033
87. LP (2) S 4	507. RY (16) C 10	0.06	3.36	0.013
87. LP (2) S 4	508. RY (17) C 10	0.09	3.31	0.016
87. LP (2) S 4	518. RY (1) H 11	0.66	1.57	0.029
87. LP (2) S 4	519. RY (2) H 11	0.08	2.46	0.012
87. LP (2) S 4	522. RY (5) H 11	0.07	3.46	0.014
87. LP (2) S 4	564. RY (11) C 14	0.09	2.73	0.014
87. LP (2) S 4	586. RY (2) C 16	0.06	1.95	0.009
87. LP (2) S 4	596. RY (12) C 16	0.08	2.66	0.013
87. LP (2) S 4	611. RY (1) C 17	1.53	2.49	0.055
87. LP (2) S 4	612. RY (2) C 17	0.16	1.78	0.015
87. LP (2) S 4	613. RY (3) C 17	0.45	1.43	0.023
87. LP (2) S 4	614. RY (4) C 17	1.89	2.80	0.065
87. LP (2) S 4	615. RY (5) C 17	0.42	3.18	0.032
87. LP (2) S 4	616. RY (6) C 17	0.76	2.56	0.039
87. LP (2) S 4	617. RY (7) C 17	0.08	2.79	0.013
87. LP (2) S 4	619. RY (9) C 17	0.08	3.07	0.014
87. LP (2) S 4	620. RY (10) C 17	0.10	3.02	0.015
87. LP (2) S 4	622. RY (12) C 17	0.61	3.45	0.041
87. LP (2) S 4	625. RY (15) C 17	0.25	4.22	0.029
87. LP (2) S 4	628. RY (18) C 17	0.22	2.73	0.022

87.	LP	(2)	S	4	631.	RY	(21)	C	17	0.07	3.68	0.014
87.	LP	(2)	S	4	695.	RY	(2)	C	21	0.05	1.84	0.009
87.	LP	(2)	S	4	699.	RY	(6)	C	21	0.05	3.83	0.012
87.	LP	(2)	S	4	704.	RY	(11)	C	21	0.16	2.72	0.018
87.	LP	(2)	S	4	720.	RY	(1)	C	22	1.26	2.33	0.048
87.	LP	(2)	S	4	721.	RY	(2)	C	22	0.51	1.89	0.028
87.	LP	(2)	S	4	722.	RY	(3)	C	22	0.79	1.56	0.031
87.	LP	(2)	S	4	723.	RY	(4)	C	22	1.85	2.68	0.063
87.	LP	(2)	S	4	724.	RY	(5)	C	22	0.28	2.67	0.024
87.	LP	(2)	S	4	726.	RY	(7)	C	22	0.48	2.59	0.031
87.	LP	(2)	S	4	730.	RY	(11)	C	22	0.89	3.73	0.052
87.	LP	(2)	S	4	731.	RY	(12)	C	22	0.26	3.41	0.026
87.	LP	(2)	S	4	732.	RY	(13)	C	22	0.14	3.23	0.019
87.	LP	(2)	S	4	734.	RY	(15)	C	22	0.17	4.56	0.025
87.	LP	(2)	S	4	735.	RY	(16)	C	22	0.09	4.17	0.018
87.	LP	(2)	S	4	737.	RY	(18)	C	22	0.07	3.57	0.014
87.	LP	(2)	S	4	740.	RY	(21)	C	22	0.10	4.09	0.018
87.	LP	(2)	S	4	749.	RY	(4)	C	23	0.06	1.72	0.009
87.	LP	(2)	S	4	786.	RY	(10)	C	25	0.08	2.54	0.013
87.	LP	(2)	S	4	808.	RY	(1)	C	27	0.88	2.13	0.039
87.	LP	(2)	S	4	810.	RY	(3)	C	27	0.20	1.67	0.016
87.	LP	(2)	S	4	811.	RY	(4)	C	27	0.97	1.91	0.038
87.	LP	(2)	S	4	813.	RY	(6)	C	27	0.46	2.27	0.029
87.	LP	(2)	S	4	815.	RY	(8)	C	27	0.72	3.33	0.044
87.	LP	(2)	S	4	816.	RY	(9)	C	27	0.31	2.75	0.026
87.	LP	(2)	S	4	817.	RY	(10)	C	27	0.18	2.66	0.019
87.	LP	(2)	S	4	818.	RY	(11)	C	27	0.17	2.68	0.019
87.	LP	(2)	S	4	819.	RY	(12)	C	27	0.06	3.46	0.013
87.	LP	(2)	S	4	823.	RY	(16)	C	27	0.31	2.82	0.027
87.	LP	(2)	S	4	834.	RY	(1)	H	28	1.56	1.86	0.048
87.	LP	(2)	S	4	835.	RY	(2)	H	28	0.14	2.57	0.017
87.	LP	(2)	S	4	838.	RY	(5)	H	28	0.09	3.55	0.016
117.	BD	(1)	Pt	1- S 2	195.	BD*	(1)	N	7- C 10	0.07	0.85	0.007
117.	BD	(1)	Pt	1- S 2	197.	BD*	(1)	N	7- C 17	0.15	0.82	0.010
117.	BD	(1)	Pt	1- S 2	199.	BD*	(1)	N	8- C 27	0.06	0.90	0.007
117.	BD	(1)	Pt	1- S 2	224.	BD*	(1)	C	27- H 28	0.05	1.10	0.007
117.	BD	(1)	Pt	1- S 2	414.	RY	(1)	N	7	4.20	4.90	0.128
117.	BD	(1)	Pt	1- S 2	415.	RY	(2)	N	7	0.68	1.44	0.028
117.	BD	(1)	Pt	1- S 2	416.	RY	(3)	N	7	0.08	1.94	0.011
117.	BD	(1)	Pt	1- S 2	417.	RY	(4)	N	7	0.74	2.71	0.040
117.	BD	(1)	Pt	1- S 2	422.	RY	(9)	N	7	0.10	4.69	0.019
117.	BD	(1)	Pt	1- S 2	424.	RY	(11)	N	7	0.09	5.12	0.019
117.	BD	(1)	Pt	1- S 2	426.	RY	(13)	N	7	0.17	4.47	0.024
117.	BD	(1)	Pt	1- S 2	427.	RY	(14)	N	7	0.06	4.45	0.015
117.	BD	(1)	Pt	1- S 2	428.	RY	(15)	N	7	0.11	4.88	0.021
117.	BD	(1)	Pt	1- S 2	440.	RY	(1)	N	8	0.58	4.84	0.047
117.	BD	(1)	Pt	1- S 2	441.	RY	(2)	N	8	0.14	1.58	0.013
117.	BD	(1)	Pt	1- S 2	442.	RY	(3)	N	8	0.31	1.92	0.022
117.	BD	(1)	Pt	1- S 2	443.	RY	(4)	N	8	1.40	2.80	0.056
117.	BD	(1)	Pt	1- S 2	446.	RY	(7)	N	8	0.06	3.75	0.014
117.	BD	(1)	Pt	1- S 2	447.	RY	(8)	N	8	0.16	3.29	0.021
117.	BD	(1)	Pt	1- S 2	448.	RY	(9)	N	8	0.28	4.73	0.033
117.	BD	(1)	Pt	1- S 2	449.	RY	(10)	N	8	0.06	4.27	0.014
117.	BD	(1)	Pt	1- S 2	451.	RY	(12)	N	8	0.33	4.06	0.033
117.	BD	(1)	Pt	1- S 2	452.	RY	(13)	N	8	0.47	3.98	0.039
117.	BD	(1)	Pt	1- S 2	453.	RY	(14)	N	8	0.06	4.86	0.015
117.	BD	(1)	Pt	1- S 2	492.	RY	(1)	C	10	0.56	2.13	0.031
117.	BD	(1)	Pt	1- S 2	493.	RY	(2)	C	10	0.19	1.59	0.015
117.	BD	(1)	Pt	1- S 2	495.	RY	(4)	C	10	0.82	1.97	0.036
117.	BD	(1)	Pt	1- S 2	497.	RY	(6)	C	10	0.06	3.73	0.013
117.	BD	(1)	Pt	1- S 2	498.	RY	(7)	C	10	0.07	1.98	0.010
117.	BD	(1)	Pt	1- S 2	499.	RY	(8)	C	10	0.53	3.16	0.037
117.	BD	(1)	Pt	1- S 2	504.	RY	(13)	C	10	0.28	3.12	0.027
117.	BD	(1)	Pt	1- S 2	508.	RY	(17)	C	10	0.07	3.55	0.014
117.	BD	(1)	Pt	1- S 2	518.	RY	(1)	H	11	0.23	1.81	0.018
117.	BD	(1)	Pt	1- S 2	519.	RY	(2)	H	11	0.08	2.69	0.013
117.	BD	(1)	Pt	1- S 2	526.	RY	(4)	C	12	0.05	1.76	0.009
117.	BD	(1)	Pt	1- S 2	564.	RY	(11)	C	14	0.07	2.96	0.013
117.	BD	(1)	Pt	1- S 2	611.	RY	(1)	C	17	1.39	2.72	0.055
117.	BD	(1)	Pt	1- S 2	613.	RY	(3)	C	17	0.15	1.66	0.014
117.	BD	(1)	Pt	1- S 2	614.	RY	(4)	C	17	0.66	3.03	0.040
117.	BD	(1)	Pt	1- S 2	615.	RY	(5)	C	17	0.30	3.41	0.029
117.	BD	(1)	Pt	1- S 2	616.	RY	(6)	C	17	0.40	2.80	0.030
117.	BD	(1)	Pt	1- S 2	622.	RY	(12)	C	17	0.30	3.69	0.030
117.	BD	(1)	Pt	1- S 2	625.	RY	(15)	C	17	0.18	4.45	0.025
117.	BD	(1)	Pt	1- S 2	628.	RY	(18)	C	17	0.08	2.96	0.014
117.	BD	(1)	Pt	1- S 2	704.	RY	(11)	C	21	0.12	2.95	0.017
117.	BD	(1)	Pt	1- S 2	720.	RY	(1)	C	22	0.37	2.56	0.028
117.	BD	(1)	Pt	1- S 2	722.	RY	(3)	C	22	0.42	1.79	0.025
117.	BD	(1)	Pt	1- S 2	723.	RY	(4)	C	22	0.90	2.92	0.046
117.	BD	(1)	Pt	1- S 2	724.	RY	(5)	C	22	0.20	2.91	0.021
117.	BD	(1)	Pt	1- S 2	726.	RY	(7)	C	22	0.24	2.82	0.023
117.	BD	(1)	Pt	1- S 2	730.	RY	(11)	C	22	0.56	3.96	0.042
117.	BD	(1)	Pt	1- S 2	731.	RY	(12)	C	22	0.13	3.64	0.019
117.	BD	(1)	Pt	1- S 2	732.	RY	(13)	C	22	0.06	3.46	0.013
117.	BD	(1)	Pt	1- S 2	734.	RY	(15)	C	22	0.07	4.79	0.017
117.	BD	(1)	Pt	1- S 2	740.	RY	(21)	C	22	0.05	4.32	0.014
117.	BD	(1)	Pt	1- S 2	808.	RY	(1)	C	27	0.35	2.37	0.026
117.	BD	(1)	Pt	1- S 2	811.	RY	(4)	C	27	0.32	2.14	0.023
117.	BD	(1)	Pt	1- S 2	813.	RY	(6)	C	27	0.21	2.50	0.021
117.	BD	(1)	Pt	1- S 2	815.	RY	(8)	C	27	0.28	3.57	0.028
117.	BD	(1)	Pt	1- S 2	816.	RY	(9)	C	27	0.15	2.99	0.019
117.	BD	(1)	Pt	1- S 2	817.	RY	(10)	C	27	0.07	2.89	0.013
117.	BD	(1)	Pt	1- S 2	823.	RY	(16)	C	27	0.24	3.05	0.024
117.	BD	(1)	Pt	1- S 2	834.	RY	(1)	H	28	0.57	2.09	0.031
117.	BD	(1)	Pt	1- S 2	835.	RY	(2)	H	28	0.10	2.80	0.015
118.	BD	(1)	Pt	1- S 3	195.	BD*	(1)	N	7- C 10	0.08	0.86	0.008
118.	BD	(1)	Pt	1- S 3	198.	BD*	(1)	N	8- C 22	0.17	0.77	0.010
118.	BD	(1)	Pt	1- S 3	199.	BD*	(1)	N	8- C 27	0.06	0.91	0.007
118.	BD	(1)	Pt	1- S 3	414.	RY	(1)	N	7	0.55	4.91	0.046
118.	BD	(1)	Pt	1- S 3	416.	RY	(3)	N	7	0.42	1.95	0.025
118.	BD	(1)	Pt	1- S 3	417.	RY	(4)	N	7	1.31	2.72	0.053
118.	BD	(1)	Pt	1- S 3	420.	RY	(7)	N	7	0.16	4.51	0.024

118.	BD	(1)Pt	1- S 3	422.	RY	(9) N 7	0.38	4.70	0.038
118.	BD	(1)Pt	1- S 3	423.	RY	(10) N 7	0.05	3.94	0.013
118.	BD	(1)Pt	1- S 3	424.	RY	(11) N 7	0.06	5.13	0.015
118.	BD	(1)Pt	1- S 3	426.	RY	(13) N 7	0.23	4.48	0.029
118.	BD	(1)Pt	1- S 3	427.	RY	(14) N 7	0.15	4.46	0.023
118.	BD	(1)Pt	1- S 3	428.	RY	(15) N 7	0.12	4.89	0.022
118.	BD	(1)Pt	1- S 3	440.	RY	(1) N 8	4.06	4.85	0.125
118.	BD	(1)Pt	1- S 3	441.	RY	(2) N 8	1.13	1.59	0.038
118.	BD	(1)Pt	1- S 3	443.	RY	(4) N 8	0.82	2.81	0.043
118.	BD	(1)Pt	1- S 3	448.	RY	(9) N 8	0.05	4.74	0.014
118.	BD	(1)Pt	1- S 3	451.	RY	(12) N 8	0.21	4.07	0.026
118.	BD	(1)Pt	1- S 3	452.	RY	(13) N 8	0.29	3.99	0.030
118.	BD	(1)Pt	1- S 3	464.	RY	(25) N 8	0.09	5.37	0.020
118.	BD	(1)Pt	1- S 3	492.	RY	(1) C 10	0.20	2.14	0.018
118.	BD	(1)Pt	1- S 3	493.	RY	(2) C 10	0.08	1.60	0.010
118.	BD	(1)Pt	1- S 3	495.	RY	(4) C 10	0.30	1.98	0.022
118.	BD	(1)Pt	1- S 3	499.	RY	(8) C 10	0.38	3.17	0.031
118.	BD	(1)Pt	1- S 3	504.	RY	(13) C 10	0.13	3.13	0.018
118.	BD	(1)Pt	1- S 3	508.	RY	(17) C 10	0.11	3.56	0.018
118.	BD	(1)Pt	1- S 3	518.	RY	(1) H 11	0.14	1.82	0.014
118.	BD	(1)Pt	1- S 3	519.	RY	(2) H 11	0.05	2.70	0.011
118.	BD	(1)Pt	1- S 3	564.	RY	(11) C 14	0.06	2.97	0.012
118.	BD	(1)Pt	1- S 3	596.	RY	(12) C 16	0.05	2.90	0.011
118.	BD	(1)Pt	1- S 3	611.	RY	(1) C 17	0.41	2.73	0.030
118.	BD	(1)Pt	1- S 3	613.	RY	(3) C 17	0.23	1.67	0.017
118.	BD	(1)Pt	1- S 3	614.	RY	(4) C 17	0.90	3.04	0.047
118.	BD	(1)Pt	1- S 3	615.	RY	(5) C 17	0.31	3.42	0.029
118.	BD	(1)Pt	1- S 3	616.	RY	(6) C 17	0.35	2.81	0.028
118.	BD	(1)Pt	1- S 3	617.	RY	(7) C 17	0.07	3.04	0.013
118.	BD	(1)Pt	1- S 3	620.	RY	(10) C 17	0.06	3.26	0.013
118.	BD	(1)Pt	1- S 3	622.	RY	(12) C 17	0.36	3.70	0.033
118.	BD	(1)Pt	1- S 3	625.	RY	(15) C 17	0.08	4.46	0.017
118.	BD	(1)Pt	1- S 3	628.	RY	(18) C 17	0.13	2.97	0.018
118.	BD	(1)Pt	1- S 3	696.	RY	(3) C 21	0.05	1.81	0.009
118.	BD	(1)Pt	1- S 3	704.	RY	(11) C 21	0.09	2.96	0.014
118.	BD	(1)Pt	1- S 3	720.	RY	(1) C 22	1.27	2.57	0.051
118.	BD	(1)Pt	1- S 3	721.	RY	(2) C 22	0.13	2.13	0.015
118.	BD	(1)Pt	1- S 3	722.	RY	(3) C 22	0.25	1.80	0.019
118.	BD	(1)Pt	1- S 3	723.	RY	(4) C 22	0.67	2.93	0.040
118.	BD	(1)Pt	1- S 3	724.	RY	(5) C 22	0.19	2.92	0.021
118.	BD	(1)Pt	1- S 3	726.	RY	(7) C 22	0.28	2.83	0.025
118.	BD	(1)Pt	1- S 3	730.	RY	(11) C 22	0.47	3.97	0.039
118.	BD	(1)Pt	1- S 3	731.	RY	(12) C 22	0.11	3.65	0.018
118.	BD	(1)Pt	1- S 3	732.	RY	(13) C 22	0.10	3.47	0.017
118.	BD	(1)Pt	1- S 3	734.	RY	(15) C 22	0.13	4.80	0.022
118.	BD	(1)Pt	1- S 3	735.	RY	(16) C 22	0.07	4.41	0.015
118.	BD	(1)Pt	1- S 3	740.	RY	(21) C 22	0.05	4.33	0.014
118.	BD	(1)Pt	1- S 3	780.	RY	(4) C 25	0.08	1.89	0.011
118.	BD	(1)Pt	1- S 3	808.	RY	(1) C 27	0.88	2.38	0.041
118.	BD	(1)Pt	1- S 3	809.	RY	(2) C 27	0.08	1.54	0.010
118.	BD	(1)Pt	1- S 3	811.	RY	(4) C 27	0.82	2.15	0.037
118.	BD	(1)Pt	1- S 3	813.	RY	(6) C 27	0.22	2.51	0.021
118.	BD	(1)Pt	1- S 3	815.	RY	(8) C 27	0.33	3.58	0.031
118.	BD	(1)Pt	1- S 3	816.	RY	(9) C 27	0.18	3.00	0.021
118.	BD	(1)Pt	1- S 3	817.	RY	(10) C 27	0.17	2.90	0.020
118.	BD	(1)Pt	1- S 3	818.	RY	(11) C 27	0.06	2.92	0.011
118.	BD	(1)Pt	1- S 3	823.	RY	(16) C 27	0.21	3.06	0.022
118.	BD	(1)Pt	1- S 3	834.	RY	(1) H 28	0.74	2.10	0.035
118.	BD	(1)Pt	1- S 3	835.	RY	(2) H 28	0.11	2.81	0.016
118.	BD	(1)Pt	1- S 3	838.	RY	(5) H 28	0.06	3.79	0.013
119.	BD	(1) S	2- C 29	414.	RY	(1) N 7	0.54	5.01	0.047
119.	BD	(1) S	2- C 29	415.	RY	(2) N 7	0.08	1.54	0.010
119.	BD	(1) S	2- C 29	440.	RY	(1) N 8	0.84	4.95	0.058
119.	BD	(1) S	2- C 29	441.	RY	(2) N 8	0.23	1.68	0.018
119.	BD	(1) S	2- C 29	443.	RY	(4) N 8	0.06	2.91	0.012
119.	BD	(1) S	2- C 29	451.	RY	(12) N 8	0.08	4.17	0.016
119.	BD	(1) S	2- C 29	452.	RY	(13) N 8	0.08	4.08	0.016
119.	BD	(1) S	2- C 29	494.	RY	(3) C 10	0.11	2.03	0.013
119.	BD	(1) S	2- C 29	495.	RY	(4) C 10	0.07	2.07	0.011
119.	BD	(1) S	2- C 29	499.	RY	(8) C 10	0.17	3.27	0.021
119.	BD	(1) S	2- C 29	504.	RY	(13) C 10	0.08	3.22	0.014
119.	BD	(1) S	2- C 29	518.	RY	(1) H 11	0.49	1.91	0.027
119.	BD	(1) S	2- C 29	611.	RY	(1) C 17	0.16	2.83	0.019
119.	BD	(1) S	2- C 29	614.	RY	(4) C 17	0.20	3.13	0.022
119.	BD	(1) S	2- C 29	616.	RY	(6) C 17	0.05	2.90	0.011
119.	BD	(1) S	2- C 29	622.	RY	(12) C 17	0.06	3.79	0.013
119.	BD	(1) S	2- C 29	720.	RY	(1) C 22	0.16	2.67	0.018
119.	BD	(1) S	2- C 29	721.	RY	(2) C 22	0.09	2.23	0.013
119.	BD	(1) S	2- C 29	722.	RY	(3) C 22	0.06	1.90	0.009
119.	BD	(1) S	2- C 29	723.	RY	(4) C 22	0.20	3.02	0.022
119.	BD	(1) S	2- C 29	726.	RY	(7) C 22	0.06	2.93	0.012
119.	BD	(1) S	2- C 29	730.	RY	(11) C 22	0.10	4.07	0.018
119.	BD	(1) S	2- C 29	808.	RY	(1) C 27	0.14	2.47	0.016
119.	BD	(1) S	2- C 29	811.	RY	(4) C 27	0.12	2.25	0.015
119.	BD	(1) S	2- C 29	813.	RY	(6) C 27	0.05	2.61	0.010
119.	BD	(1) S	2- C 29	815.	RY	(8) C 27	0.08	3.67	0.015
119.	BD	(1) S	2- C 29	834.	RY	(1) H 28	0.25	2.20	0.021
120.	BD	(1) S	2- C 44	414.	RY	(1) N 7	0.84	5.02	0.058
120.	BD	(1) S	2- C 44	415.	RY	(2) N 7	0.15	1.55	0.013
120.	BD	(1) S	2- C 44	416.	RY	(3) N 7	0.06	2.06	0.010
120.	BD	(1) S	2- C 44	417.	RY	(4) N 7	0.15	2.83	0.019
120.	BD	(1) S	2- C 44	426.	RY	(13) N 7	0.07	4.59	0.016
120.	BD	(1) S	2- C 44	428.	RY	(15) N 7	0.06	4.99	0.015
120.	BD	(1) S	2- C 44	440.	RY	(1) N 8	1.52	4.96	0.077
120.	BD	(1) S	2- C 44	441.	RY	(2) N 8	0.19	1.69	0.016
120.	BD	(1) S	2- C 44	443.	RY	(4) N 8	0.09	2.92	0.015
120.	BD	(1) S	2- C 44	451.	RY	(12) N 8	0.15	4.18	0.022
120.	BD	(1) S	2- C 44	452.	RY	(13) N 8	0.20	4.09	0.025
120.	BD	(1) S	2- C 44	492.	RY	(1) C 10	0.16	2.25	0.017
120.	BD	(1) S	2- C 44	495.	RY	(4) C 10	0.21	2.08	0.019
120.	BD	(1) S	2- C 44	499.	RY	(8) C 10	0.13	3.28	0.019
120.	BD	(1) S	2- C 44	518.	RY	(1) H 11	0.09	1.92	0.012
120.	BD	(1) S	2- C 44	519.	RY	(2) H 11	0.06	2.81	0.011

120.	BD	(1)	S	2-	C	44	611.	RY	(1)	C	17	0.27	2.84	0.025
120.	BD	(1)	S	2-	C	44	613.	RY	(3)	C	17	0.09	1.78	0.012
120.	BD	(1)	S	2-	C	44	614.	RY	(4)	C	17	0.42	3.14	0.033
120.	BD	(1)	S	2-	C	44	615.	RY	(5)	C	17	0.10	3.52	0.016
120.	BD	(1)	S	2-	C	44	616.	RY	(6)	C	17	0.12	2.91	0.017
120.	BD	(1)	S	2-	C	44	622.	RY	(12)	C	17	0.15	3.80	0.021
120.	BD	(1)	S	2-	C	44	625.	RY	(15)	C	17	0.05	4.57	0.014
120.	BD	(1)	S	2-	C	44	720.	RY	(1)	C	22	0.32	2.68	0.026
120.	BD	(1)	S	2-	C	44	721.	RY	(2)	C	22	0.13	2.24	0.015
120.	BD	(1)	S	2-	C	44	722.	RY	(3)	C	22	0.11	1.91	0.013
120.	BD	(1)	S	2-	C	44	723.	RY	(4)	C	22	0.37	3.03	0.030
120.	BD	(1)	S	2-	C	44	724.	RY	(5)	C	22	0.06	3.02	0.012
120.	BD	(1)	S	2-	C	44	726.	RY	(7)	C	22	0.10	2.94	0.015
120.	BD	(1)	S	2-	C	44	730.	RY	(11)	C	22	0.18	4.08	0.024
120.	BD	(1)	S	2-	C	44	808.	RY	(1)	C	27	0.22	2.48	0.021
120.	BD	(1)	S	2-	C	44	810.	RY	(3)	C	27	0.05	2.02	0.009
120.	BD	(1)	S	2-	C	44	811.	RY	(4)	C	27	0.18	2.26	0.018
120.	BD	(1)	S	2-	C	44	813.	RY	(6)	C	27	0.09	2.62	0.013
120.	BD	(1)	S	2-	C	44	815.	RY	(8)	C	27	0.15	3.68	0.021
120.	BD	(1)	S	2-	C	44	816.	RY	(9)	C	27	0.06	3.10	0.012
120.	BD	(1)	S	2-	C	44	823.	RY	(16)	C	27	0.06	3.16	0.012
120.	BD	(1)	S	2-	C	44	834.	RY	(1)	H	28	0.36	2.21	0.025
121.	BD	(1)	S	3-	C	32	414.	RY	(1)	N	7	1.25	5.02	0.071
121.	BD	(1)	S	3-	C	32	415.	RY	(2)	N	7	0.30	1.55	0.019
121.	BD	(1)	S	3-	C	32	417.	RY	(4)	N	7	0.06	2.83	0.012
121.	BD	(1)	S	3-	C	32	424.	RY	(11)	N	7	0.06	5.23	0.016
121.	BD	(1)	S	3-	C	32	426.	RY	(13)	N	7	0.07	4.58	0.016
121.	BD	(1)	S	3-	C	32	428.	RY	(15)	N	7	0.06	4.99	0.015
121.	BD	(1)	S	3-	C	32	440.	RY	(1)	N	8	0.86	4.95	0.058
121.	BD	(1)	S	3-	C	32	441.	RY	(2)	N	8	0.20	1.69	0.016
121.	BD	(1)	S	3-	C	32	443.	RY	(4)	N	8	0.08	2.92	0.013
121.	BD	(1)	S	3-	C	32	451.	RY	(12)	N	8	0.08	4.18	0.017
121.	BD	(1)	S	3-	C	32	452.	RY	(13)	N	8	0.13	4.09	0.021
121.	BD	(1)	S	3-	C	32	492.	RY	(1)	C	10	0.13	2.24	0.015
121.	BD	(1)	S	3-	C	32	495.	RY	(4)	C	10	0.19	2.08	0.018
121.	BD	(1)	S	3-	C	32	499.	RY	(8)	C	10	0.15	3.27	0.020
121.	BD	(1)	S	3-	C	32	504.	RY	(13)	C	10	0.06	3.23	0.013
121.	BD	(1)	S	3-	C	32	518.	RY	(1)	H	11	0.16	1.92	0.015
121.	BD	(1)	S	3-	C	32	611.	RY	(1)	C	17	0.27	2.83	0.025
121.	BD	(1)	S	3-	C	32	612.	RY	(2)	C	17	0.06	2.12	0.010
121.	BD	(1)	S	3-	C	32	613.	RY	(3)	C	17	0.06	1.77	0.009
121.	BD	(1)	S	3-	C	32	614.	RY	(4)	C	17	0.30	3.14	0.028
121.	BD	(1)	S	3-	C	32	615.	RY	(5)	C	17	0.10	3.52	0.017
121.	BD	(1)	S	3-	C	32	616.	RY	(6)	C	17	0.15	2.91	0.018
121.	BD	(1)	S	3-	C	32	622.	RY	(12)	C	17	0.10	3.80	0.017
121.	BD	(1)	S	3-	C	32	720.	RY	(1)	C	22	0.20	2.68	0.021
121.	BD	(1)	S	3-	C	32	721.	RY	(2)	C	22	0.14	2.23	0.016
121.	BD	(1)	S	3-	C	32	722.	RY	(3)	C	22	0.10	1.90	0.012
121.	BD	(1)	S	3-	C	32	723.	RY	(4)	C	22	0.32	3.03	0.028
121.	BD	(1)	S	3-	C	32	726.	RY	(7)	C	22	0.07	2.93	0.012
121.	BD	(1)	S	3-	C	32	730.	RY	(11)	C	22	0.14	4.07	0.022
121.	BD	(1)	S	3-	C	32	810.	RY	(3)	C	27	0.14	2.01	0.015
121.	BD	(1)	S	3-	C	32	811.	RY	(4)	C	27	0.12	2.26	0.015
121.	BD	(1)	S	3-	C	32	813.	RY	(6)	C	27	0.09	2.61	0.014
121.	BD	(1)	S	3-	C	32	815.	RY	(8)	C	27	0.18	3.68	0.023
121.	BD	(1)	S	3-	C	32	817.	RY	(10)	C	27	0.06	3.00	0.012
121.	BD	(1)	S	3-	C	32	834.	RY	(1)	H	28	0.78	2.21	0.037
122.	BD	(1)	S	3-	C	35	414.	RY	(1)	N	7	0.86	5.02	0.058
122.	BD	(1)	S	3-	C	35	440.	RY	(1)	N	8	0.50	4.95	0.045
122.	BD	(1)	S	3-	C	35	441.	RY	(2)	N	8	0.13	1.69	0.013
122.	BD	(1)	S	3-	C	35	443.	RY	(4)	N	8	0.08	2.92	0.014
122.	BD	(1)	S	3-	C	35	451.	RY	(12)	N	8	0.07	4.18	0.015
122.	BD	(1)	S	3-	C	35	452.	RY	(13)	N	8	0.08	4.09	0.017
122.	BD	(1)	S	3-	C	35	492.	RY	(1)	C	10	0.07	2.24	0.011
122.	BD	(1)	S	3-	C	35	495.	RY	(4)	C	10	0.09	2.08	0.012
122.	BD	(1)	S	3-	C	35	499.	RY	(8)	C	10	0.07	3.27	0.013
122.	BD	(1)	S	3-	C	35	518.	RY	(1)	H	11	0.08	1.92	0.011
122.	BD	(1)	S	3-	C	35	611.	RY	(1)	C	17	0.18	2.83	0.020
122.	BD	(1)	S	3-	C	35	614.	RY	(4)	C	17	0.21	3.14	0.023
122.	BD	(1)	S	3-	C	35	615.	RY	(5)	C	17	0.06	3.52	0.013
122.	BD	(1)	S	3-	C	35	616.	RY	(6)	C	17	0.09	2.91	0.015
122.	BD	(1)	S	3-	C	35	622.	RY	(12)	C	17	0.07	3.80	0.014
122.	BD	(1)	S	3-	C	35	720.	RY	(1)	C	22	0.13	2.68	0.017
122.	BD	(1)	S	3-	C	35	721.	RY	(2)	C	22	0.07	2.24	0.011
122.	BD	(1)	S	3-	C	35	722.	RY	(3)	C	22	0.07	1.90	0.010
122.	BD	(1)	S	3-	C	35	723.	RY	(4)	C	22	0.19	3.03	0.021
122.	BD	(1)	S	3-	C	35	730.	RY	(11)	C	22	0.10	4.07	0.018
122.	BD	(1)	S	3-	C	35	808.	RY	(1)	C	27	0.10	2.48	0.014
122.	BD	(1)	S	3-	C	35	811.	RY	(4)	C	27	0.10	2.26	0.014
122.	BD	(1)	S	3-	C	35	813.	RY	(6)	C	27	0.07	2.61	0.012
122.	BD	(1)	S	3-	C	35	815.	RY	(8)	C	27	0.09	3.68	0.016
122.	BD	(1)	S	3-	C	35	834.	RY	(1)	H	28	0.27	2.21	0.022
161.	BD	(1)	C	32-	H	33	414.	RY	(1)	N	7	0.07	4.97	0.017
161.	BD	(1)	C	32-	H	33	440.	RY	(1)	N	8	0.06	4.91	0.016
161.	BD	(1)	C	32-	H	33	834.	RY	(1)	H	28	0.05	2.16	0.009
171.	BD	(1)	C	44-	H	45	414.	RY	(1)	N	7	0.05	5.00	0.014
from unit 1 to unit 3							240.	BD*	(1)	Sb	47-cl 51	0.70	0.53	0.017
80.	LP	(1)	Pt	1			1059.	RY	(5)	Sb	47	0.14	1.70	0.014
80.	LP	(1)	Pt	1			1060.	RY	(6)	Sb	47	0.11	1.22	0.010
80.	LP	(1)	Pt	1			1061.	RY	(7)	Sb	47	0.56	1.66	0.027
80.	LP	(1)	Pt	1			1064.	RY	(10)	Sb	47	0.20	2.43	0.020
80.	LP	(1)	Pt	1			1066.	RY	(12)	Sb	47	1.26	1.75	0.042
80.	LP	(1)	Pt	1			1067.	RY	(13)	Sb	47	2.06	1.73	0.053
80.	LP	(1)	Pt	1			1070.	RY	(16)	Sb	47	2.96	5.07	0.109
80.	LP	(1)	Pt	1			1071.	RY	(17)	Sb	47	0.73	2.16	0.035
80.	LP	(1)	Pt	1			1072.	RY	(18)	Sb	47	0.11	2.27	0.014
80.	LP	(1)	Pt	1			1075.	RY	(21)	Sb	47	0.38	3.02	0.030
80.	LP	(1)	Pt	1			1077.	RY	(23)	Sb	47	0.14	2.13	0.016
80.	LP	(1)	Pt	1			1080.	RY	(26)	Sb	47	0.18	4.41	0.025
80.	LP	(1)	Pt	1			1082.	RY	(28)	Sb	47	0.07	2.63	0.012
80.	LP	(1)	Pt	1			1083.	RY	(29)	Sb	47	0.54	33.92	0.121

80. LP (1)Pt 1	1084. RY (30)Sb 47	0.29	5.44	0.036
80. LP (1)Pt 1	1085. RY (31)Sb 47	0.21	2.11	0.019
80. LP (1)Pt 1	1086. RY (32)Sb 47	0.08	33.46	0.047
80. LP (1)Pt 1	1176. RY (1)Cl 51	0.17	1.77	0.016
80. LP (1)Pt 1	1177. RY (2)Cl 51	0.12	2.62	0.016
80. LP (1)Pt 1	1181. RY (6)Cl 51	0.23	1.91	0.019
80. LP (1)Pt 1	1185. RY (10)Cl 51	0.15	3.67	0.021
80. LP (1)Pt 1	1193. RY (18)Cl 51	0.09	3.28	0.015
81. LP (2)Pt 1	183. LV (2)Sb 47	0.10	0.55	0.007
81. LP (2)Pt 1	1058. RY (4)Sb 47	0.16	1.13	0.012
82. LP (3)Pt 1	240. BD* (1)Sb 47-C1 51	0.16	0.62	0.009
82. LP (3)Pt 1	1066. RY (12)Sb 47	0.05	1.83	0.009
82. LP (3)Pt 1	1067. RY (13)Sb 47	0.11	1.81	0.012
82. LP (3)Pt 1	1070. RY (16)Sb 47	0.18	5.16	0.027
83. LP (4)Pt 1	240. BD* (1)Sb 47-C1 51	0.21	0.59	0.010
83. LP (4)Pt 1	1064. RY (10)Sb 47	0.12	2.50	0.016
83. LP (4)Pt 1	1066. RY (12)Sb 47	0.17	1.81	0.016
83. LP (4)Pt 1	1067. RY (13)Sb 47	0.15	1.79	0.015
83. LP (4)Pt 1	1070. RY (16)Sb 47	0.09	5.13	0.020
84. LP (1) S 2	183. LV (2)Sb 47	0.05	0.59	0.005
87. LP (2) S 4	240. BD* (1)Sb 47-C1 51	0.46	0.39	0.012
87. LP (2) S 4	1055. RY (1)Sb 47	0.07	1.17	0.008
87. LP (2) S 4	1061. RY (7)Sb 47	0.05	1.52	0.008
87. LP (2) S 4	1064. RY (10)Sb 47	0.14	2.29	0.016
87. LP (2) S 4	1065. RY (11)Sb 47	0.07	2.54	0.012
87. LP (2) S 4	1066. RY (12)Sb 47	0.26	1.60	0.018
87. LP (2) S 4	1067. RY (13)Sb 47	0.32	1.59	0.020
87. LP (2) S 4	1070. RY (16)Sb 47	0.25	4.93	0.031
117. BD (1)Pt 1- S 2	183. LV (2)Sb 47	0.09	0.58	0.006
117. BD (1)Pt 1- S 2	240. BD* (1)Sb 47-C1 51	0.64	0.62	0.018
117. BD (1)Pt 1- S 2	1061. RY (7)Sb 47	0.08	1.75	0.011
117. BD (1)Pt 1- S 2	1066. RY (12)Sb 47	0.07	1.84	0.010
117. BD (1)Pt 1- S 2	1067. RY (13)Sb 47	0.09	1.82	0.011
117. BD (1)Pt 1- S 2	1070. RY (16)Sb 47	0.30	5.16	0.035
118. BD (1)Pt 1- S 3	182. LV (1)Sb 47	0.17	0.59	0.009
118. BD (1)Pt 1- S 3	240. BD* (1)Sb 47-C1 51	0.51	0.63	0.016
118. BD (1)Pt 1- S 3	1061. RY (7)Sb 47	0.10	1.77	0.012
118. BD (1)Pt 1- S 3	1067. RY (13)Sb 47	0.12	1.83	0.013
118. BD (1)Pt 1- S 3	1070. RY (16)Sb 47	0.27	5.17	0.034
119. BD (1) S 2- C 29	1066. RY (12)Sb 47	0.05	1.94	0.009
119. BD (1) S 2- C 29	1067. RY (13)Sb 47	0.05	1.92	0.009
119. BD (1) S 2- C 29	1070. RY (16)Sb 47	0.06	5.26	0.016
120. BD (1) S 2- C 44	1061. RY (7)Sb 47	0.06	1.87	0.009
120. BD (1) S 2- C 44	1066. RY (12)Sb 47	0.08	1.95	0.011
120. BD (1) S 2- C 44	1067. RY (13)Sb 47	0.08	1.93	0.011
120. BD (1) S 2- C 44	1070. RY (16)Sb 47	0.12	5.28	0.022
121. BD (1) S 3- C 32	1066. RY (12)Sb 47	0.07	1.95	0.010
121. BD (1) S 3- C 32	1067. RY (13)Sb 47	0.10	1.93	0.012
121. BD (1) S 3- C 32	1070. RY (16)Sb 47	0.08	5.27	0.018
122. BD (1) S 3- C 35	1070. RY (16)Sb 47	0.07	5.27	0.017
from unit 1 to unit 4				
80. LP (1)Pt 1	1092. RY (1)Cl 48	0.57	1.20	0.023
80. LP (1)Pt 1	1093. RY (2)Cl 48	0.25	1.63	0.018
80. LP (1)Pt 1	1096. RY (5)Cl 48	0.15	1.73	0.014
80. LP (1)Pt 1	1097. RY (6)Cl 48	0.14	1.43	0.013
80. LP (1)Pt 1	1098. RY (7)Cl 48	0.79	2.02	0.036
80. LP (1)Pt 1	1100. RY (9)Cl 48	0.59	1.41	0.026
80. LP (1)Pt 1	1101. RY (10)Cl 48	0.05	3.22	0.011
80. LP (1)Pt 1	1118. RY (27)Cl 48	0.12	2.29	0.015
82. LP (3)Pt 1	1098. RY (7)Cl 48	0.07	2.11	0.011
87. LP (2) S 4	1092. RY (1)Cl 48	0.07	1.06	0.008
87. LP (2) S 4	1098. RY (7)Cl 48	0.10	1.88	0.012
87. LP (2) S 4	1100. RY (9)Cl 48	0.07	1.27	0.009
from unit 1 to unit 5				
80. LP (1)Pt 1	1122. RY (3)Cl 49	0.11	1.20	0.010
80. LP (1)Pt 1	1123. RY (4)Cl 49	0.16	1.21	0.012
80. LP (1)Pt 1	1124. RY (5)Cl 49	0.13	2.24	0.015
80. LP (1)Pt 1	1126. RY (7)Cl 49	0.08	1.68	0.010
80. LP (1)Pt 1	1127. RY (8)Cl 49	0.25	2.90	0.024
80. LP (1)Pt 1	1134. RY (15)Cl 49	0.07	3.85	0.014
80. LP (1)Pt 1	1135. RY (16)Cl 49	0.07	3.30	0.013
80. LP (1)Pt 1	1136. RY (17)Cl 49	0.06	3.24	0.013
84. LP (1) S 2	1128. RY (9)Cl 49	0.15	1.60	0.014
161. BD (1) C 32- H 33	1123. RY (4)Cl 49	0.06	1.37	0.008
161. BD (1) C 32- H 33	1125. RY (6)Cl 49	0.07	1.59	0.009
from unit 1 to unit 6				
80. LP (1)Pt 1	1148. RY (1)Cl 50	0.66	1.22	0.025
80. LP (1)Pt 1	1151. RY (4)Cl 50	0.23	1.22	0.015
80. LP (1)Pt 1	1153. RY (6)Cl 50	0.63	1.63	0.029
80. LP (1)Pt 1	1154. RY (7)Cl 50	1.41	1.72	0.044
80. LP (1)Pt 1	1155. RY (8)Cl 50	1.51	2.64	0.056
80. LP (1)Pt 1	1156. RY (9)Cl 50	0.84	1.79	0.035
80. LP (1)Pt 1	1158. RY (11)Cl 50	0.08	3.40	0.015
80. LP (1)Pt 1	1163. RY (16)Cl 50	0.10	2.62	0.014
80. LP (1)Pt 1	1166. RY (19)Cl 50	0.12	2.81	0.016
82. LP (3)Pt 1	1153. RY (6)Cl 50	0.08	1.71	0.011
82. LP (3)Pt 1	1154. RY (7)Cl 50	0.06	1.80	0.009
82. LP (3)Pt 1	1155. RY (8)Cl 50	0.08	2.72	0.013
82. LP (3)Pt 1	1156. RY (9)Cl 50	0.05	1.88	0.009
83. LP (4)Pt 1	1154. RY (7)Cl 50	0.08	1.78	0.010
83. LP (4)Pt 1	1155. RY (8)Cl 50	0.09	2.70	0.014
83. LP (4)Pt 1	1156. RY (9)Cl 50	0.07	1.85	0.010
85. LP (1) S 3	1156. RY (9)Cl 50	0.09	1.89	0.012
87. LP (2) S 4	1148. RY (1)Cl 50	0.07	1.08	0.008
87. LP (2) S 4	1153. RY (6)Cl 50	0.09	1.49	0.010
87. LP (2) S 4	1154. RY (7)Cl 50	0.17	1.57	0.014
87. LP (2) S 4	1155. RY (8)Cl 50	0.15	2.49	0.017
117. BD (1)Pt 1- S 2	1154. RY (7)Cl 50	0.06	1.81	0.009
117. BD (1)Pt 1- S 2	1155. RY (8)Cl 50	0.05	2.73	0.011
118. BD (1)Pt 1- S 3	1148. RY (1)Cl 50	0.08	1.32	0.009

118. BD (1)Pt 1- S 3	1154. RY (7)C1 50	0.09	1.82	0.011
118. BD (1)Pt 1- S 3	1155. RY (8)C1 50	0.10	2.74	0.015
118. BD (1)Pt 1- S 3	1156. RY (9)C1 50	0.12	1.89	0.013
161. BD (1) C 32- H 33	1153. RY (6)C1 50	0.07	1.78	0.010
from unit 1 to unit 7				
80. LP (1)Pt 1	1204. RY (1)C1 52	0.57	1.25	0.024
80. LP (1)Pt 1	1205. RY (2)C1 52	0.94	1.93	0.038
80. LP (1)Pt 1	1206. RY (3)C1 52	0.11	1.21	0.010
80. LP (1)Pt 1	1207. RY (4)C1 52	0.07	1.20	0.008
80. LP (1)Pt 1	1208. RY (5)C1 52	0.26	2.67	0.024
80. LP (1)Pt 1	1209. RY (6)C1 52	0.11	1.53	0.012
80. LP (1)Pt 1	1210. RY (7)C1 52	0.19	2.37	0.019
80. LP (1)Pt 1	1214. RY (11)C1 52	0.09	4.41	0.018
80. LP (1)Pt 1	1216. RY (13)C1 52	0.09	3.59	0.016
80. LP (1)Pt 1	1231. RY (28)C1 52	0.12	2.78	0.016
82. LP (3)Pt 1	1205. RY (2)C1 52	0.06	2.01	0.010
87. LP (2) S 4	1204. RY (1)C1 52	0.07	1.11	0.008
87. LP (2) S 4	1205. RY (2)C1 52	0.10	1.79	0.012
from unit 1 to unit 8				
80. LP (1)Pt 1	1233. RY (2) N 53	0.16	1.31	0.013
80. LP (1)Pt 1	1234. RY (3) N 53	0.09	1.33	0.010
80. LP (1)Pt 1	1239. RY (8) N 53	0.07	2.31	0.012
80. LP (1)Pt 1	1262. RY (5) C 54	0.06	3.20	0.012
80. LP (1)Pt 1	1264. RY (7) C 54	0.07	2.29	0.011
80. LP (1)Pt 1	1284. RY (1) C 55	0.09	1.43	0.010
80. LP (1)Pt 1	1287. RY (4) C 55	0.14	1.73	0.014
80. LP (1)Pt 1	1291. RY (8) C 55	0.05	2.81	0.011
from unit 2 to unit 1				
92. LP (1) N 7	184. BD*(1)Pt 1- S 2	3.72	0.61	0.042
92. LP (1) N 7	185. BD*(1)Pt 1- S 3	73.14	0.61	0.189
92. LP (1) N 7	186. BD*(1) S 2- C 29	0.06	0.54	0.005
92. LP (1) N 7	248. RY (1)Pt 1	5.17	2.39	0.099
92. LP (1) N 7	249. RY (2)Pt 1	8.67	2.97	0.143
92. LP (1) N 7	250. RY (3)Pt 1	1.87	3.02	0.067
92. LP (1) N 7	251. RY (4)Pt 1	0.11	2.46	0.015
92. LP (1) N 7	252. RY (5)Pt 1	7.10	2.93	0.129
92. LP (1) N 7	253. RY (6)Pt 1	0.40	3.38	0.033
92. LP (1) N 7	255. RY (8)Pt 1	9.05	2.85	0.143
92. LP (1) N 7	256. RY (9)Pt 1	5.96	2.93	0.118
92. LP (1) N 7	257. RY (10)Pt 1	10.19	4.71	0.196
92. LP (1) N 7	258. RY (11)Pt 1	3.46	3.04	0.092
92. LP (1) N 7	259. RY (12)Pt 1	2.51	3.02	0.078
92. LP (1) N 7	260. RY (13)Pt 1	8.69	7.61	0.230
92. LP (1) N 7	261. RY (14)Pt 1	0.32	2.57	0.026
92. LP (1) N 7	262. RY (15)Pt 1	6.85	3.41	0.136
92. LP (1) N 7	263. RY (16)Pt 1	4.51	3.21	0.107
92. LP (1) N 7	265. RY (18)Pt 1	2.48	3.94	0.088
92. LP (1) N 7	266. RY (19)Pt 1	2.10	3.91	0.081
92. LP (1) N 7	267. RY (20)Pt 1	4.47	4.42	0.125
92. LP (1) N 7	268. RY (21)Pt 1	0.17	3.00	0.020
92. LP (1) N 7	269. RY (22)Pt 1	0.56	2.51	0.033
92. LP (1) N 7	270. RY (23)Pt 1	0.51	2.40	0.031
92. LP (1) N 7	271. RY (24)Pt 1	5.17	5.16	0.146
92. LP (1) N 7	272. RY (25)Pt 1	0.41	2.55	0.029
92. LP (1) N 7	273. RY (26)Pt 1	13.42	37.26	0.631
92. LP (1) N 7	274. RY (27)Pt 1	0.41	27.52	0.095
92. LP (1) N 7	276. RY (29)Pt 1	4.23	236.96	0.894
92. LP (1) N 7	278. RY (1) S 2	0.16	1.34	0.013
92. LP (1) N 7	279. RY (2) S 2	2.49	1.64	0.057
92. LP (1) N 7	280. RY (3) S 2	0.37	1.32	0.020
92. LP (1) N 7	281. RY (4) S 2	3.56	1.89	0.073
92. LP (1) N 7	282. RY (5) S 2	9.30	5.35	0.199
92. LP (1) N 7	283. RY (6) S 2	4.69	2.05	0.087
92. LP (1) N 7	284. RY (7) S 2	1.29	2.13	0.047
92. LP (1) N 7	285. RY (8) S 2	1.17	2.23	0.046
92. LP (1) N 7	286. RY (9) S 2	1.49	2.52	0.055
92. LP (1) N 7	287. RY (10) S 2	0.48	2.34	0.030
92. LP (1) N 7	289. RY (12) S 2	0.67	3.38	0.042
92. LP (1) N 7	292. RY (15) S 2	0.20	2.57	0.020
92. LP (1) N 7	293. RY (16) S 2	0.94	3.31	0.050
92. LP (1) N 7	294. RY (17) S 2	0.71	3.42	0.044
92. LP (1) N 7	295. RY (18) S 2	0.11	3.55	0.018
92. LP (1) N 7	297. RY (20) S 2	1.29	3.87	0.063
92. LP (1) N 7	298. RY (21) S 2	0.18	3.16	0.021
92. LP (1) N 7	299. RY (22) S 2	2.58	4.73	0.099
92. LP (1) N 7	300. RY (23) S 2	0.23	2.92	0.023
92. LP (1) N 7	304. RY (27) S 2	0.09	7.14	0.023
92. LP (1) N 7	306. RY (1) S 3	0.12	1.43	0.012
92. LP (1) N 7	307. RY (2) S 3	0.74	1.37	0.028
92. LP (1) N 7	308. RY (3) S 3	0.19	1.37	0.015
92. LP (1) N 7	309. RY (4) S 3	3.74	1.77	0.073
92. LP (1) N 7	310. RY (5) S 3	7.39	3.97	0.153
92. LP (1) N 7	311. RY (6) S 3	10.60	4.09	0.186
92. LP (1) N 7	312. RY (7) S 3	2.08	2.30	0.062
92. LP (1) N 7	313. RY (8) S 3	0.66	2.06	0.033
92. LP (1) N 7	314. RY (9) S 3	0.75	2.32	0.037
92. LP (1) N 7	315. RY (10) S 3	0.78	2.37	0.038
92. LP (1) N 7	317. RY (12) S 3	1.00	3.37	0.052
92. LP (1) N 7	318. RY (13) S 3	0.07	2.66	0.012
92. LP (1) N 7	321. RY (16) S 3	0.18	3.34	0.022
92. LP (1) N 7	322. RY (17) S 3	1.65	3.87	0.071
92. LP (1) N 7	323. RY (18) S 3	0.81	3.43	0.047
92. LP (1) N 7	325. RY (20) S 3	2.15	3.91	0.082
92. LP (1) N 7	326. RY (21) S 3	0.40	3.36	0.033
92. LP (1) N 7	327. RY (22) S 3	2.36	3.30	0.079
92. LP (1) N 7	328. RY (23) S 3	0.23	2.96	0.024
92. LP (1) N 7	332. RY (27) S 3	0.18	11.60	0.041
92. LP (1) N 7	334. RY (1) S 4	1.16	1.42	0.036
92. LP (1) N 7	335. RY (2) S 4	0.32	1.46	0.019
92. LP (1) N 7	340. RY (7) S 4	0.20	1.69	0.016

92. LP (1) N 7	341. RY (8) S 4	0.37	1.95	0.024
92. LP (1) N 7	342. RY (9) S 4	0.29	2.08	0.022
92. LP (1) N 7	348. RY (15) S 4	0.43	2.69	0.031
92. LP (1) N 7	349. RY (16) S 4	0.13	2.87	0.017
92. LP (1) N 7	350. RY (17) S 4	0.40	3.12	0.031
92. LP (1) N 7	353. RY (20) S 4	0.06	3.93	0.014
92. LP (1) N 7	356. RY (23) S 4	0.15	3.71	0.021
92. LP (1) N 7	357. RY (24) S 4	0.18	3.89	0.023
92. LP (1) N 7	839. RY (1) C 29	0.31	1.80	0.021
92. LP (1) N 7	840. RY (2) C 29	1.81	1.56	0.047
92. LP (1) N 7	842. RY (4) C 29	1.32	2.12	0.047
92. LP (1) N 7	843. RY (5) C 29	0.85	2.29	0.039
92. LP (1) N 7	844. RY (6) C 29	0.05	2.48	0.010
92. LP (1) N 7	845. RY (7) C 29	0.19	1.73	0.016
92. LP (1) N 7	847. RY (9) C 29	0.06	3.08	0.012
92. LP (1) N 7	849. RY (11) C 29	0.38	2.47	0.027
92. LP (1) N 7	850. RY (12) C 29	0.59	3.45	0.040
92. LP (1) N 7	851. RY (13) C 29	0.26	3.22	0.026
92. LP (1) N 7	853. RY (15) C 29	0.09	3.36	0.016
92. LP (1) N 7	855. RY (17) C 29	0.08	3.71	0.015
92. LP (1) N 7	858. RY (20) C 29	0.06	3.71	0.014
92. LP (1) N 7	867. RY (3) H 30	0.07	2.68	0.012
92. LP (1) N 7	870. RY (1) H 31	0.08	1.79	0.011
92. LP (1) N 7	874. RY (5) H 31	0.07	3.18	0.013
92. LP (1) N 7	875. RY (1) C 32	1.53	1.75	0.046
92. LP (1) N 7	878. RY (4) C 32	1.29	2.18	0.047
92. LP (1) N 7	880. RY (6) C 32	0.40	1.89	0.025
92. LP (1) N 7	881. RY (7) C 32	0.41	2.03	0.026
92. LP (1) N 7	882. RY (8) C 32	0.12	2.74	0.016
92. LP (1) N 7	883. RY (9) C 32	0.22	3.04	0.023
92. LP (1) N 7	884. RY (10) C 32	0.05	2.79	0.011
92. LP (1) N 7	885. RY (11) C 32	0.76	2.66	0.040
92. LP (1) N 7	886. RY (12) C 32	0.12	3.35	0.018
92. LP (1) N 7	887. RY (13) C 32	0.13	3.46	0.019
92. LP (1) N 7	889. RY (15) C 32	0.42	4.27	0.038
92. LP (1) N 7	901. RY (1) H 33	0.15	1.94	0.015
92. LP (1) N 7	902. RY (2) H 33	0.20	2.54	0.020
92. LP (1) N 7	905. RY (5) H 33	0.11	2.85	0.016
92. LP (1) N 7	911. RY (1) C 35	1.85	1.69	0.050
92. LP (1) N 7	912. RY (2) C 35	0.47	2.20	0.029
92. LP (1) N 7	913. RY (3) C 35	0.05	1.72	0.008
92. LP (1) N 7	914. RY (4) C 35	2.05	2.18	0.060
92. LP (1) N 7	915. RY (5) C 35	0.56	2.20	0.031
92. LP (1) N 7	917. RY (7) C 35	0.22	2.09	0.019
92. LP (1) N 7	918. RY (8) C 35	0.46	2.38	0.030
92. LP (1) N 7	919. RY (9) C 35	0.06	3.37	0.012
92. LP (1) N 7	920. RY (10) C 35	0.24	2.47	0.022
92. LP (1) N 7	921. RY (11) C 35	0.53	2.71	0.034
92. LP (1) N 7	922. RY (12) C 35	0.05	4.01	0.013
92. LP (1) N 7	923. RY (13) C 35	0.71	4.09	0.048
92. LP (1) N 7	924. RY (14) C 35	0.11	4.54	0.020
92. LP (1) N 7	927. RY (17) C 35	0.07	3.39	0.014
92. LP (1) N 7	928. RY (18) C 35	0.12	3.86	0.019
92. LP (1) N 7	933. RY (23) C 35	0.05	3.90	0.013
92. LP (1) N 7	937. RY (1) H 36	0.09	1.61	0.011
92. LP (1) N 7	942. RY (1) H 37	0.19	1.71	0.016
92. LP (1) N 7	945. RY (4) H 37	0.08	3.11	0.014
92. LP (1) N 7	948. RY (2) C 38	0.30	1.96	0.022
92. LP (1) N 7	950. RY (4) C 38	0.09	1.69	0.011
92. LP (1) N 7	952. RY (6) C 38	0.74	2.02	0.034
92. LP (1) N 7	957. RY (11) C 38	0.08	2.95	0.013
92. LP (1) N 7	959. RY (13) C 38	0.46	2.85	0.032
92. LP (1) N 7	962. RY (16) C 38	0.12	3.10	0.017
92. LP (1) N 7	973. RY (1) H 39	0.75	1.72	0.032
92. LP (1) N 7	975. RY (3) H 39	0.26	2.94	0.025
92. LP (1) N 7	978. RY (1) H 40	0.08	1.78	0.011
92. LP (1) N 7	988. RY (6) C 41	0.50	2.39	0.031
92. LP (1) N 7	989. RY (7) C 41	0.18	1.94	0.017
92. LP (1) N 7	991. RY (9) C 41	0.28	2.83	0.025
92. LP (1) N 7	992. RY (10) C 41	0.07	3.90	0.015
92. LP (1) N 7	993. RY (11) C 41	0.23	3.10	0.024
92. LP (1) N 7	996. RY (14) C 41	0.14	3.25	0.019
92. LP (1) N 7	998. RY (16) C 41	0.08	3.63	0.015
92. LP (1) N 7	1009. RY (1) H 42	0.13	1.47	0.012
92. LP (1) N 7	1019. RY (1) C 44	0.73	1.68	0.031
92. LP (1) N 7	1020. RY (2) C 44	0.30	2.08	0.022
92. LP (1) N 7	1021. RY (3) C 44	0.12	1.85	0.014
92. LP (1) N 7	1022. RY (4) C 44	1.87	2.09	0.056
92. LP (1) N 7	1024. RY (6) C 44	0.36	2.14	0.025
92. LP (1) N 7	1025. RY (7) C 44	0.09	2.63	0.014
92. LP (1) N 7	1027. RY (9) C 44	0.38	2.68	0.028
92. LP (1) N 7	1028. RY (10) C 44	0.14	3.17	0.019
92. LP (1) N 7	1029. RY (11) C 44	1.00	2.88	0.048
92. LP (1) N 7	1030. RY (12) C 44	0.08	3.21	0.014
92. LP (1) N 7	1031. RY (13) C 44	0.35	4.68	0.036
92. LP (1) N 7	1032. RY (14) C 44	0.06	3.21	0.012
92. LP (1) N 7	1034. RY (16) C 44	0.12	4.31	0.020
92. LP (1) N 7	1036. RY (18) C 44	0.09	4.05	0.017
92. LP (1) N 7	1045. RY (1) H 45	0.43	1.75	0.024
92. LP (1) N 7	1046. RY (2) H 45	0.11	2.82	0.016
92. LP (1) N 7	1048. RY (4) H 45	0.09	3.00	0.015
92. LP (1) N 7	1050. RY (1) H 46	0.26	1.65	0.018
92. LP (1) N 7	1053. RY (4) H 46	0.06	2.77	0.011
93. LP (1) N 8	184. BD* (1) Pt 1- S 2	78.43	0.60	0.194
93. LP (1) N 8	185. BD* (1) Pt 1- S 3	3.81	0.61	0.043
93. LP (1) N 8	248. RY (1) Pt 1	7.18	2.38	0.117
93. LP (1) N 8	249. RY (2) Pt 1	10.22	2.97	0.156
93. LP (1) N 8	250. RY (3) Pt 1	2.30	3.02	0.074
93. LP (1) N 8	252. RY (5) Pt 1	6.92	2.92	0.127
93. LP (1) N 8	253. RY (6) Pt 1	2.02	3.38	0.074
93. LP (1) N 8	254. RY (7) Pt 1	0.95	2.23	0.041
93. LP (1) N 8	255. RY (8) Pt 1	7.41	2.84	0.130
93. LP (1) N 8	256. RY (9) Pt 1	3.65	2.93	0.092

93. LP (1) N 8	257. RY (10) Pt 1	14.16	4.71	0.230
93. LP (1) N 8	258. RY (11) Pt 1	2.06	3.04	0.071
93. LP (1) N 8	259. RY (12) Pt 1	4.69	3.02	0.106
93. LP (1) N 8	260. RY (13) Pt 1	9.55	7.60	0.241
93. LP (1) N 8	261. RY (14) Pt 1	1.74	2.57	0.060
93. LP (1) N 8	262. RY (15) Pt 1	6.35	3.40	0.131
93. LP (1) N 8	263. RY (16) Pt 1	5.22	3.20	0.115
93. LP (1) N 8	264. RY (17) Pt 1	1.40	2.70	0.055
93. LP (1) N 8	265. RY (18) Pt 1	3.72	3.93	0.108
93. LP (1) N 8	266. RY (19) Pt 1	2.47	3.90	0.088
93. LP (1) N 8	267. RY (20) Pt 1	3.97	4.42	0.118
93. LP (1) N 8	268. RY (21) Pt 1	0.43	2.99	0.032
93. LP (1) N 8	269. RY (22) Pt 1	0.59	2.50	0.034
93. LP (1) N 8	270. RY (23) Pt 1	1.03	2.39	0.044
93. LP (1) N 8	271. RY (24) Pt 1	5.83	5.16	0.155
93. LP (1) N 8	272. RY (25) Pt 1	0.97	2.54	0.044
93. LP (1) N 8	273. RY (26) Pt 1	15.00	37.26	0.667
93. LP (1) N 8	274. RY (27) Pt 1	0.41	27.51	0.095
93. LP (1) N 8	276. RY (29) Pt 1	4.76	236.96	0.948
93. LP (1) N 8	278. RY (1) S 2	0.21	1.34	0.015
93. LP (1) N 8	279. RY (2) S 2	1.73	1.63	0.047
93. LP (1) N 8	280. RY (3) S 2	0.39	1.32	0.020
93. LP (1) N 8	281. RY (4) S 2	5.95	1.89	0.095
93. LP (1) N 8	282. RY (5) S 2	10.25	5.35	0.209
93. LP (1) N 8	283. RY (6) S 2	6.76	2.04	0.105
93. LP (1) N 8	284. RY (7) S 2	1.92	2.12	0.057
93. LP (1) N 8	285. RY (8) S 2	2.22	2.23	0.063
93. LP (1) N 8	286. RY (9) S 2	1.91	2.52	0.062
93. LP (1) N 8	287. RY (10) S 2	0.65	2.33	0.035
93. LP (1) N 8	289. RY (12) S 2	0.98	3.37	0.051
93. LP (1) N 8	292. RY (15) S 2	0.35	2.57	0.027
93. LP (1) N 8	293. RY (16) S 2	0.82	3.31	0.047
93. LP (1) N 8	294. RY (17) S 2	1.20	3.42	0.057
93. LP (1) N 8	295. RY (18) S 2	0.19	3.55	0.023
93. LP (1) N 8	297. RY (20) S 2	1.71	3.87	0.073
93. LP (1) N 8	298. RY (21) S 2	0.16	3.15	0.020
93. LP (1) N 8	299. RY (22) S 2	3.05	4.73	0.107
93. LP (1) N 8	300. RY (23) S 2	0.24	2.91	0.024
93. LP (1) N 8	304. RY (27) S 2	0.11	7.13	0.025
93. LP (1) N 8	306. RY (1) S 3	0.07	1.43	0.009
93. LP (1) N 8	307. RY (2) S 3	1.75	1.36	0.044
93. LP (1) N 8	308. RY (3) S 3	0.70	1.37	0.028
93. LP (1) N 8	309. RY (4) S 3	3.51	1.77	0.070
93. LP (1) N 8	310. RY (5) S 3	9.20	3.97	0.171
93. LP (1) N 8	311. RY (6) S 3	10.23	4.09	0.183
93. LP (1) N 8	312. RY (7) S 3	1.97	2.29	0.060
93. LP (1) N 8	313. RY (8) S 3	0.29	2.06	0.022
93. LP (1) N 8	314. RY (9) S 3	0.71	2.32	0.036
93. LP (1) N 8	315. RY (10) S 3	0.76	2.37	0.038
93. LP (1) N 8	317. RY (12) S 3	0.90	3.37	0.049
93. LP (1) N 8	318. RY (13) S 3	0.20	2.65	0.020
93. LP (1) N 8	321. RY (16) S 3	0.12	3.33	0.018
93. LP (1) N 8	322. RY (17) S 3	1.52	3.87	0.069
93. LP (1) N 8	323. RY (18) S 3	1.09	3.42	0.055
93. LP (1) N 8	325. RY (20) S 3	2.24	3.91	0.083
93. LP (1) N 8	326. RY (21) S 3	0.53	3.36	0.038
93. LP (1) N 8	327. RY (22) S 3	2.44	3.29	0.080
93. LP (1) N 8	328. RY (23) S 3	0.31	2.96	0.027
93. LP (1) N 8	329. RY (24) S 3	0.15	7.18	0.029
93. LP (1) N 8	334. RY (1) S 4	1.56	1.42	0.042
93. LP (1) N 8	335. RY (2) S 4	0.34	1.45	0.020
93. LP (1) N 8	340. RY (7) S 4	0.13	1.69	0.013
93. LP (1) N 8	341. RY (8) S 4	0.56	1.95	0.029
93. LP (1) N 8	342. RY (9) S 4	0.32	2.08	0.023
93. LP (1) N 8	348. RY (15) S 4	0.50	2.69	0.033
93. LP (1) N 8	349. RY (16) S 4	0.09	2.87	0.014
93. LP (1) N 8	350. RY (17) S 4	0.53	3.11	0.036
93. LP (1) N 8	353. RY (20) S 4	0.06	3.93	0.014
93. LP (1) N 8	356. RY (23) S 4	0.18	3.71	0.023
93. LP (1) N 8	357. RY (24) S 4	0.21	3.89	0.026
93. LP (1) N 8	839. RY (1) C 29	0.39	1.80	0.024
93. LP (1) N 8	840. RY (2) C 29	2.23	1.56	0.053
93. LP (1) N 8	842. RY (4) C 29	1.30	2.11	0.047
93. LP (1) N 8	843. RY (5) C 29	1.19	2.29	0.047
93. LP (1) N 8	844. RY (6) C 29	0.08	2.48	0.013
93. LP (1) N 8	845. RY (7) C 29	0.19	1.72	0.016
93. LP (1) N 8	847. RY (9) C 29	0.06	3.08	0.012
93. LP (1) N 8	849. RY (11) C 29	0.45	2.47	0.030
93. LP (1) N 8	850. RY (12) C 29	0.77	3.45	0.046
93. LP (1) N 8	851. RY (13) C 29	0.34	3.21	0.029
93. LP (1) N 8	853. RY (15) C 29	0.09	3.36	0.015
93. LP (1) N 8	855. RY (17) C 29	0.11	3.70	0.018
93. LP (1) N 8	858. RY (20) C 29	0.07	3.71	0.015
93. LP (1) N 8	867. RY (3) H 30	0.09	2.68	0.014
93. LP (1) N 8	870. RY (1) H 31	0.10	1.79	0.012
93. LP (1) N 8	874. RY (5) H 31	0.09	3.18	0.015
93. LP (1) N 8	875. RY (1) C 32	1.58	1.74	0.047
93. LP (1) N 8	878. RY (4) C 32	1.58	2.17	0.052
93. LP (1) N 8	879. RY (5) C 32	0.09	2.06	0.012
93. LP (1) N 8	880. RY (6) C 32	0.39	1.88	0.024
93. LP (1) N 8	881. RY (7) C 32	0.41	2.03	0.026
93. LP (1) N 8	882. RY (8) C 32	0.07	2.74	0.013
93. LP (1) N 8	883. RY (9) C 32	0.23	3.04	0.024
93. LP (1) N 8	885. RY (11) C 32	0.77	2.66	0.040
93. LP (1) N 8	886. RY (12) C 32	0.16	3.35	0.020
93. LP (1) N 8	887. RY (13) C 32	0.13	3.46	0.019
93. LP (1) N 8	889. RY (15) C 32	0.40	4.27	0.037
93. LP (1) N 8	901. RY (1) H 33	0.17	1.94	0.016
93. LP (1) N 8	902. RY (2) H 33	0.24	2.53	0.022
93. LP (1) N 8	905. RY (5) H 33	0.11	2.85	0.016
93. LP (1) N 8	911. RY (1) C 35	1.73	1.69	0.048
93. LP (1) N 8	912. RY (2) C 35	0.56	2.20	0.031
93. LP (1) N 8	913. RY (3) C 35	0.07	1.71	0.010

93.	LP	(1)	N	8	914.	RY	(4)	C	35	2.52	2.18	0.066
93.	LP	(1)	N	8	915.	RY	(5)	C	35	0.45	2.19	0.028
93.	LP	(1)	N	8	917.	RY	(7)	C	35	0.29	2.09	0.022
93.	LP	(1)	N	8	918.	RY	(8)	C	35	0.44	2.38	0.029
93.	LP	(1)	N	8	920.	RY	(10)	C	35	0.22	2.47	0.021
93.	LP	(1)	N	8	921.	RY	(11)	C	35	0.59	2.70	0.036
93.	LP	(1)	N	8	923.	RY	(13)	C	35	0.70	4.08	0.048
93.	LP	(1)	N	8	924.	RY	(14)	C	35	0.13	4.53	0.022
93.	LP	(1)	N	8	927.	RY	(17)	C	35	0.07	3.39	0.014
93.	LP	(1)	N	8	928.	RY	(18)	C	35	0.11	3.85	0.019
93.	LP	(1)	N	8	933.	RY	(23)	C	35	0.06	3.90	0.014
93.	LP	(1)	N	8	937.	RY	(1)	H	36	0.11	1.61	0.012
93.	LP	(1)	N	8	942.	RY	(1)	H	37	0.21	1.71	0.017
93.	LP	(1)	N	8	945.	RY	(4)	H	37	0.08	3.10	0.014
93.	LP	(1)	N	8	948.	RY	(2)	C	38	0.43	1.96	0.026
93.	LP	(1)	N	8	950.	RY	(4)	C	38	0.06	1.69	0.009
93.	LP	(1)	N	8	952.	RY	(6)	C	38	0.87	2.01	0.037
93.	LP	(1)	N	8	953.	RY	(7)	C	38	0.06	2.25	0.010
93.	LP	(1)	N	8	957.	RY	(11)	C	38	0.07	2.94	0.013
93.	LP	(1)	N	8	959.	RY	(13)	C	38	0.52	2.84	0.034
93.	LP	(1)	N	8	962.	RY	(16)	C	38	0.12	3.09	0.017
93.	LP	(1)	N	8	973.	RY	(1)	H	39	0.71	1.71	0.031
93.	LP	(1)	N	8	975.	RY	(3)	H	39	0.26	2.93	0.025
93.	LP	(1)	N	8	978.	RY	(1)	H	40	0.07	1.78	0.010
93.	LP	(1)	N	8	988.	RY	(6)	C	41	0.53	2.38	0.032
93.	LP	(1)	N	8	989.	RY	(7)	C	41	0.19	1.94	0.017
93.	LP	(1)	N	8	991.	RY	(9)	C	41	0.29	2.82	0.026
93.	LP	(1)	N	8	992.	RY	(10)	C	41	0.08	3.90	0.015
93.	LP	(1)	N	8	993.	RY	(11)	C	41	0.27	3.10	0.026
93.	LP	(1)	N	8	996.	RY	(14)	C	41	0.14	3.24	0.019
93.	LP	(1)	N	8	998.	RY	(16)	C	41	0.09	3.63	0.016
93.	LP	(1)	N	8	1009.	RY	(1)	H	42	0.13	1.47	0.012
93.	LP	(1)	N	8	1019.	RY	(1)	C	44	1.00	1.68	0.037
93.	LP	(1)	N	8	1020.	RY	(2)	C	44	0.28	2.07	0.021
93.	LP	(1)	N	8	1021.	RY	(3)	C	44	0.10	1.84	0.012
93.	LP	(1)	N	8	1022.	RY	(4)	C	44	2.12	2.09	0.059
93.	LP	(1)	N	8	1024.	RY	(6)	C	44	0.45	2.14	0.028
93.	LP	(1)	N	8	1025.	RY	(7)	C	44	0.18	2.62	0.019
93.	LP	(1)	N	8	1027.	RY	(9)	C	44	0.45	2.67	0.031
93.	LP	(1)	N	8	1028.	RY	(10)	C	44	0.16	3.16	0.020
93.	LP	(1)	N	8	1029.	RY	(11)	C	44	1.29	2.88	0.054
93.	LP	(1)	N	8	1030.	RY	(12)	C	44	0.09	3.20	0.015
93.	LP	(1)	N	8	1031.	RY	(13)	C	44	0.42	4.68	0.039
93.	LP	(1)	N	8	1032.	RY	(14)	C	44	0.09	3.21	0.015
93.	LP	(1)	N	8	1034.	RY	(16)	C	44	0.13	4.30	0.021
93.	LP	(1)	N	8	1035.	RY	(17)	C	44	0.07	3.13	0.013
93.	LP	(1)	N	8	1036.	RY	(18)	C	44	0.11	4.05	0.019
93.	LP	(1)	N	8	1045.	RY	(1)	H	45	0.59	1.74	0.029
93.	LP	(1)	N	8	1046.	RY	(2)	H	45	0.13	2.81	0.017
93.	LP	(1)	N	8	1048.	RY	(4)	H	45	0.10	3.00	0.016
93.	LP	(1)	N	8	1049.	RY	(5)	H	45	0.06	3.11	0.013
93.	LP	(1)	N	8	1050.	RY	(1)	H	46	0.29	1.64	0.020
93.	LP	(1)	N	8	1053.	RY	(4)	H	46	0.08	2.77	0.013
128.	BD	(1)	N	7- C 10	184.	BD*	(1)	Pt	1- S 2	0.08	1.00	0.008
128.	BD	(1)	N	7- C 10	185.	BD*	(1)	Pt	1- S 3	1.81	1.01	0.038
128.	BD	(1)	N	7- C 10	250.	RY	(3)	Pt	1	0.24	3.42	0.025
128.	BD	(1)	N	7- C 10	251.	RY	(4)	Pt	1	0.35	2.86	0.028
128.	BD	(1)	N	7- C 10	253.	RY	(6)	Pt	1	0.30	3.78	0.030
128.	BD	(1)	N	7- C 10	254.	RY	(7)	Pt	1	0.05	2.64	0.011
128.	BD	(1)	N	7- C 10	259.	RY	(12)	Pt	1	0.09	3.42	0.016
128.	BD	(1)	N	7- C 10	267.	RY	(20)	Pt	1	0.21	4.82	0.028
128.	BD	(1)	N	7- C 10	268.	RY	(21)	Pt	1	0.07	3.39	0.014
128.	BD	(1)	N	7- C 10	272.	RY	(25)	Pt	1	0.06	2.95	0.011
128.	BD	(1)	N	7- C 10	274.	RY	(27)	Pt	1	0.16	27.92	0.059
128.	BD	(1)	N	7- C 10	275.	RY	(28)	Pt	1	0.11	28.49	0.050
129.	BD	(2)	N	7- C 10	184.	BD*	(1)	Pt	1- S 2	0.06	0.50	0.005
129.	BD	(2)	N	7- C 10	185.	BD*	(1)	Pt	1- S 3	0.18	0.51	0.008
129.	BD	(2)	N	7- C 10	248.	RY	(1)	Pt	1	0.08	2.28	0.012
129.	BD	(2)	N	7- C 10	252.	RY	(5)	Pt	1	0.63	2.82	0.038
129.	BD	(2)	N	7- C 10	254.	RY	(7)	Pt	1	0.19	2.13	0.018
129.	BD	(2)	N	7- C 10	255.	RY	(8)	Pt	1	0.06	2.74	0.012
129.	BD	(2)	N	7- C 10	267.	RY	(20)	Pt	1	0.06	4.32	0.014
129.	BD	(2)	N	7- C 10	269.	RY	(22)	Pt	1	0.10	2.40	0.014
129.	BD	(2)	N	7- C 10	270.	RY	(23)	Pt	1	0.06	2.29	0.011
129.	BD	(2)	N	7- C 10	273.	RY	(26)	Pt	1	0.05	37.15	0.039
130.	BD	(1)	N	7- C 17	184.	BD*	(1)	Pt	1- S 2	0.49	1.00	0.020
130.	BD	(1)	N	7- C 17	185.	BD*	(1)	Pt	1- S 3	3.77	1.00	0.055
130.	BD	(1)	N	7- C 17	248.	RY	(1)	Pt	1	0.19	2.78	0.020
130.	BD	(1)	N	7- C 17	249.	RY	(2)	Pt	1	0.95	3.36	0.050
130.	BD	(1)	N	7- C 17	250.	RY	(3)	Pt	1	0.09	3.41	0.016
130.	BD	(1)	N	7- C 17	251.	RY	(4)	Pt	1	0.16	2.85	0.019
130.	BD	(1)	N	7- C 17	252.	RY	(5)	Pt	1	0.21	3.32	0.023
130.	BD	(1)	N	7- C 17	254.	RY	(7)	Pt	1	0.12	2.63	0.016
130.	BD	(1)	N	7- C 17	255.	RY	(8)	Pt	1	0.38	3.24	0.031
130.	BD	(1)	N	7- C 17	256.	RY	(9)	Pt	1	0.07	3.32	0.014
130.	BD	(1)	N	7- C 17	257.	RY	(10)	Pt	1	0.08	5.10	0.018
130.	BD	(1)	N	7- C 17	260.	RY	(13)	Pt	1	0.18	8.00	0.034
130.	BD	(1)	N	7- C 17	262.	RY	(15)	Pt	1	0.26	3.80	0.028
130.	BD	(1)	N	7- C 17	263.	RY	(16)	Pt	1	0.11	3.60	0.018
130.	BD	(1)	N	7- C 17	265.	RY	(18)	Pt	1	0.16	4.33	0.023
130.	BD	(1)	N	7- C 17	267.	RY	(20)	Pt	1	0.35	4.81	0.037
130.	BD	(1)	N	7- C 17	269.	RY	(22)	Pt	1	0.05	2.90	0.011
130.	BD	(1)	N	7- C 17	271.	RY	(24)	Pt	1	0.22	5.55	0.031
130.	BD	(1)	N	7- C 17	273.	RY	(26)	Pt	1	0.47	37.65	0.118
130.	BD	(1)	N	7- C 17	275.	RY	(28)	Pt	1	0.09	28.48	0.045
130.	BD	(1)	N	7- C 17	276.	RY	(29)	Pt	1	0.08	237.35	0.120
130.	BD	(1)	N	7- C 17	281.	RY	(4)	S	2	0.20	2.28	0.019
130.	BD	(1)	N	7- C 17	282.	RY	(5)	S	2	0.27	5.74	0.035
130.	BD	(1)	N	7- C 17	283.	RY	(6)	S	2	0.21	2.44	0.020
130.	BD	(1)	N	7- C 17	284.	RY	(7)	S	2	0.08	2.52	0.012
130.	BD	(1)	N	7- C 17	286.	RY	(9)	S	2	0.10	2.91	0.015
130.	BD	(1)	N	7- C 17	297.	RY	(20)	S	2	0.07	4.26	0.015
130.	BD	(1)	N	7- C 17	299.	RY	(22)	S	2	0.11	5.12	0.021

130.	BD	(1)	N	7-	C	17	309.	RY	(4)	S	3	0.17	2.16	0.017
130.	BD	(1)	N	7-	C	17	310.	RY	(5)	S	3	0.38	4.36	0.036
130.	BD	(1)	N	7-	C	17	311.	RY	(6)	S	3	0.43	4.48	0.039
130.	BD	(1)	N	7-	C	17	312.	RY	(7)	S	3	0.07	2.69	0.012
130.	BD	(1)	N	7-	C	17	313.	RY	(8)	S	3	0.05	2.45	0.010
130.	BD	(1)	N	7-	C	17	327.	RY	(22)	S	3	0.08	3.69	0.016
130.	BD	(1)	N	7-	C	17	840.	RY	(2)	C	29	0.06	1.95	0.010
130.	BD	(1)	N	7-	C	17	875.	RY	(1)	C	32	0.09	2.14	0.012
130.	BD	(1)	N	7-	C	17	911.	RY	(1)	C	35	0.07	2.08	0.010
130.	BD	(1)	N	7-	C	17	914.	RY	(4)	C	35	0.06	2.57	0.011
130.	BD	(1)	N	7-	C	17	952.	RY	(6)	C	38	0.06	2.41	0.010
130.	BD	(1)	N	7-	C	17	1022.	RY	(4)	C	44	0.08	2.48	0.013
130.	BD	(1)	N	7-	C	17	1045.	RY	(1)	H	45	0.06	2.14	0.010
131.	BD	(1)	N	8-	C	22	184.	BD*	(1)	Pt	1- S 2	3.31	0.95	0.050
131.	BD	(1)	N	8-	C	22	185.	BD*	(1)	Pt	1- S 3	0.41	0.95	0.018
131.	BD	(1)	N	8-	C	22	248.	RY	(1)	Pt	1	0.17	2.73	0.019
131.	BD	(1)	N	8-	C	22	249.	RY	(2)	Pt	1	0.80	3.31	0.046
131.	BD	(1)	N	8-	C	22	251.	RY	(4)	Pt	1	0.09	2.80	0.014
131.	BD	(1)	N	8-	C	22	252.	RY	(5)	Pt	1	0.18	3.27	0.022
131.	BD	(1)	N	8-	C	22	253.	RY	(6)	Pt	1	0.07	3.72	0.015
131.	BD	(1)	N	8-	C	22	254.	RY	(7)	Pt	1	0.09	2.58	0.014
131.	BD	(1)	N	8-	C	22	255.	RY	(8)	Pt	1	0.26	3.19	0.026
131.	BD	(1)	N	8-	C	22	257.	RY	(10)	Pt	1	0.10	5.05	0.020
131.	BD	(1)	N	8-	C	22	259.	RY	(12)	Pt	1	0.08	3.36	0.015
131.	BD	(1)	N	8-	C	22	260.	RY	(13)	Pt	1	0.17	7.95	0.033
131.	BD	(1)	N	8-	C	22	262.	RY	(15)	Pt	1	0.20	3.75	0.025
131.	BD	(1)	N	8-	C	22	263.	RY	(16)	Pt	1	0.09	3.55	0.016
131.	BD	(1)	N	8-	C	22	265.	RY	(18)	Pt	1	0.23	4.28	0.028
131.	BD	(1)	N	8-	C	22	266.	RY	(19)	Pt	1	0.16	4.25	0.023
131.	BD	(1)	N	8-	C	22	267.	RY	(20)	Pt	1	0.08	4.76	0.017
131.	BD	(1)	N	8-	C	22	269.	RY	(22)	Pt	1	0.06	2.85	0.011
131.	BD	(1)	N	8-	C	22	271.	RY	(24)	Pt	1	0.21	5.50	0.030
131.	BD	(1)	N	8-	C	22	273.	RY	(26)	Pt	1	0.33	37.60	0.099
131.	BD	(1)	N	8-	C	22	276.	RY	(29)	Pt	1	0.06	237.30	0.102
131.	BD	(1)	N	8-	C	22	281.	RY	(4)	S	2	0.16	2.23	0.017
131.	BD	(1)	N	8-	C	22	282.	RY	(5)	S	2	0.31	5.69	0.038
131.	BD	(1)	N	8-	C	22	283.	RY	(6)	S	2	0.15	2.39	0.017
131.	BD	(1)	N	8-	C	22	285.	RY	(8)	S	2	0.10	2.57	0.014
131.	BD	(1)	N	8-	C	22	299.	RY	(22)	S	2	0.06	5.07	0.016
131.	BD	(1)	N	8-	C	22	309.	RY	(4)	S	3	0.10	2.11	0.013
131.	BD	(1)	N	8-	C	22	310.	RY	(5)	S	3	0.18	4.31	0.025
131.	BD	(1)	N	8-	C	22	311.	RY	(6)	S	3	0.30	4.43	0.033
131.	BD	(1)	N	8-	C	22	322.	RY	(17)	S	3	0.05	4.21	0.014
131.	BD	(1)	N	8-	C	22	325.	RY	(20)	S	3	0.05	4.25	0.013
131.	BD	(1)	N	8-	C	22	327.	RY	(22)	S	3	0.07	3.64	0.014
131.	BD	(1)	N	8-	C	22	840.	RY	(2)	C	29	0.07	1.90	0.010
131.	BD	(1)	N	8-	C	22	875.	RY	(1)	C	32	0.05	2.09	0.010
131.	BD	(1)	N	8-	C	22	911.	RY	(1)	C	35	0.05	2.03	0.009
131.	BD	(1)	N	8-	C	22	914.	RY	(4)	C	35	0.07	2.52	0.012
131.	BD	(1)	N	8-	C	22	1022.	RY	(4)	C	44	0.06	2.43	0.011
132.	BD	(1)	N	8-	C	27	184.	BD*	(1)	Pt	1- S 2	2.41	1.04	0.045
132.	BD	(1)	N	8-	C	27	185.	BD*	(1)	Pt	1- S 3	0.13	1.04	0.010
132.	BD	(1)	N	8-	C	27	250.	RY	(3)	Pt	1	0.45	3.45	0.035
132.	BD	(1)	N	8-	C	27	251.	RY	(4)	Pt	1	0.29	2.89	0.026
132.	BD	(1)	N	8-	C	27	255.	RY	(8)	Pt	1	0.10	3.28	0.016
132.	BD	(1)	N	8-	C	27	256.	RY	(9)	Pt	1	0.06	3.36	0.012
132.	BD	(1)	N	8-	C	27	257.	RY	(10)	Pt	1	0.08	5.14	0.018
132.	BD	(1)	N	8-	C	27	259.	RY	(12)	Pt	1	0.08	3.45	0.015
132.	BD	(1)	N	8-	C	27	265.	RY	(18)	Pt	1	0.18	4.37	0.025
132.	BD	(1)	N	8-	C	27	266.	RY	(19)	Pt	1	0.21	4.34	0.027
132.	BD	(1)	N	8-	C	27	268.	RY	(21)	Pt	1	0.18	3.43	0.022
132.	BD	(1)	N	8-	C	27	271.	RY	(24)	Pt	1	0.07	5.59	0.018
132.	BD	(1)	N	8-	C	27	274.	RY	(27)	Pt	1	0.13	27.95	0.054
132.	BD	(1)	N	8-	C	27	275.	RY	(28)	Pt	1	0.13	28.52	0.055
133.	BD	(2)	N	8-	C	27	184.	BD*	(1)	Pt	1- S 2	0.11	0.51	0.007
133.	BD	(2)	N	8-	C	27	185.	BD*	(1)	Pt	1- S 3	0.12	0.51	0.007
133.	BD	(2)	N	8-	C	27	248.	RY	(1)	Pt	1	0.15	2.29	0.016
133.	BD	(2)	N	8-	C	27	252.	RY	(5)	Pt	1	0.82	2.83	0.043
133.	BD	(2)	N	8-	C	27	256.	RY	(9)	Pt	1	0.09	2.83	0.014
133.	BD	(2)	N	8-	C	27	260.	RY	(13)	Pt	1	0.06	7.51	0.018
133.	BD	(2)	N	8-	C	27	261.	RY	(14)	Pt	1	0.19	2.47	0.019
133.	BD	(2)	N	8-	C	27	266.	RY	(19)	Pt	1	0.09	3.81	0.016
133.	BD	(2)	N	8-	C	27	269.	RY	(22)	Pt	1	0.08	2.41	0.013
133.	BD	(2)	N	8-	C	27	270.	RY	(23)	Pt	1	0.12	2.30	0.015
133.	BD	(2)	N	8-	C	27	273.	RY	(26)	Pt	1	0.10	37.16	0.053
133.	BD	(2)	N	8-	C	27	282.	RY	(5)	S	2	0.09	5.25	0.019
133.	BD	(2)	N	8-	C	27	310.	RY	(5)	S	3	0.09	3.87	0.017
133.	BD	(2)	N	8-	C	27	311.	RY	(6)	S	3	0.07	3.99	0.015
135.	BD	(1)	C	10-	H	11	184.	BD*	(1)	Pt	1- S 2	0.69	0.72	0.020
135.	BD	(1)	C	10-	H	11	185.	BD*	(1)	Pt	1- S 3	0.82	0.72	0.022
135.	BD	(1)	C	10-	H	11	186.	BD*	(1)	S	2- C 29	0.08	0.65	0.007
135.	BD	(1)	C	10-	H	11	248.	RY	(1)	Pt	1	0.42	2.50	0.029
135.	BD	(1)	C	10-	H	11	249.	RY	(2)	Pt	1	0.30	3.09	0.027
135.	BD	(1)	C	10-	H	11	252.	RY	(5)	Pt	1	0.50	3.04	0.035
135.	BD	(1)	C	10-	H	11	253.	RY	(6)	Pt	1	0.14	3.49	0.019
135.	BD	(1)	C	10-	H	11	255.	RY	(8)	Pt	1	0.41	2.96	0.031
135.	BD	(1)	C	10-	H	11	256.	RY	(9)	Pt	1	0.28	3.04	0.026
135.	BD	(1)	C	10-	H	11	257.	RY	(10)	Pt	1	0.73	4.83	0.053
135.	BD	(1)	C	10-	H	11	258.	RY	(11)	Pt	1	0.12	3.15	0.018
135.	BD	(1)	C	10-	H	11	259.	RY	(12)	Pt	1	0.18	3.13	0.021
135.	BD	(1)	C	10-	H	11	260.	RY	(13)	Pt	1	0.57	7.72	0.059
135.	BD	(1)	C	10-	H	11	261.	RY	(14)	Pt	1	0.10	2.68	0.015
135.	BD	(1)	C	10-	H	11	262.	RY	(15)	Pt	1	0.54	3.52	0.039
135.	BD	(1)	C	10-	H	11	263.	RY	(16)	Pt	1	0.32	3.32	0.029
135.	BD	(1)	C	10-	H	11	264.	RY	(17)	Pt	1	0.10	2.82	0.015
135.	BD	(1)	C	10-	H	11	265.	RY	(18)	Pt	1	0.18	4.05	0.024
135.	BD	(1)	C	10-	H	11	266.	RY	(19)	Pt	1	0.09	4.02	0.017
135.	BD	(1)	C	10-	H	11	267.	RY	(20)	Pt	1	0.61	4.53	0.047
135.	BD	(1)	C	10-	H	11	270.	RY	(23)	Pt	1	0.10	2.51	0.014
135.	BD	(1)	C	10-	H	11	271.	RY	(24)	Pt	1	0.35	5.27	0.038
135.	BD	(1)	C	10-	H	11	273.	RY	(26)	Pt	1	1.15	37.37	0.185
135.	BD	(1)	C	10-	H	11	275.	RY	(28)	Pt	1	0.06	28.20	0.035
135.	BD	(1)	C	10-	H	11	276.	RY	(29)	Pt	1	0.36	237.07	0.261

135. BD (1) C 10- H 11	279. RY (2) S 2	0.23	1.75	0.018
135. BD (1) C 10- H 11	281. RY (4) S 2	0.39	2.01	0.025
135. BD (1) C 10- H 11	282. RY (5) S 2	0.74	5.46	0.057
135. BD (1) C 10- H 11	283. RY (6) S 2	0.66	2.16	0.034
135. BD (1) C 10- H 11	284. RY (7) S 2	0.12	2.24	0.015
135. BD (1) C 10- H 11	285. RY (8) S 2	0.13	2.34	0.016
135. BD (1) C 10- H 11	286. RY (9) S 2	0.19	2.63	0.020
135. BD (1) C 10- H 11	289. RY (12) S 2	0.14	3.49	0.020
135. BD (1) C 10- H 11	293. RY (16) S 2	0.08	3.43	0.014
135. BD (1) C 10- H 11	294. RY (17) S 2	0.11	3.54	0.018
135. BD (1) C 10- H 11	297. RY (20) S 2	0.20	3.99	0.025
135. BD (1) C 10- H 11	299. RY (22) S 2	0.27	4.84	0.033
135. BD (1) C 10- H 11	307. RY (2) S 3	0.10	1.48	0.011
135. BD (1) C 10- H 11	308. RY (3) S 3	0.07	1.49	0.009
135. BD (1) C 10- H 11	309. RY (4) S 3	0.35	1.89	0.023
135. BD (1) C 10- H 11	310. RY (5) S 3	0.80	4.09	0.051
135. BD (1) C 10- H 11	311. RY (6) S 3	0.93	4.21	0.056
135. BD (1) C 10- H 11	312. RY (7) S 3	0.17	2.41	0.018
135. BD (1) C 10- H 11	314. RY (9) S 3	0.07	2.43	0.011
135. BD (1) C 10- H 11	315. RY (10) S 3	0.07	2.49	0.012
135. BD (1) C 10- H 11	317. RY (12) S 3	0.05	3.48	0.012
135. BD (1) C 10- H 11	322. RY (17) S 3	0.11	3.99	0.019
135. BD (1) C 10- H 11	323. RY (18) S 3	0.07	3.54	0.014
135. BD (1) C 10- H 11	325. RY (20) S 3	0.14	4.03	0.021
135. BD (1) C 10- H 11	327. RY (22) S 3	0.17	3.41	0.022
135. BD (1) C 10- H 11	334. RY (1) S 4	0.12	1.53	0.012
135. BD (1) C 10- H 11	840. RY (2) C 29	0.15	1.67	0.014
135. BD (1) C 10- H 11	842. RY (4) C 29	0.09	2.23	0.013
135. BD (1) C 10- H 11	843. RY (5) C 29	0.10	2.40	0.013
135. BD (1) C 10- H 11	850. RY (12) C 29	0.05	3.56	0.012
135. BD (1) C 10- H 11	875. RY (1) C 32	0.12	1.86	0.013
135. BD (1) C 10- H 11	878. RY (4) C 32	0.11	2.29	0.014
135. BD (1) C 10- H 11	885. RY (11) C 32	0.06	2.77	0.012
135. BD (1) C 10- H 11	911. RY (1) C 35	0.14	1.80	0.014
135. BD (1) C 10- H 11	914. RY (4) C 35	0.19	2.29	0.018
135. BD (1) C 10- H 11	923. RY (13) C 35	0.05	4.20	0.013
135. BD (1) C 10- H 11	952. RY (6) C 38	0.08	2.13	0.011
135. BD (1) C 10- H 11	973. RY (1) H 39	0.06	1.83	0.009
135. BD (1) C 10- H 11	1019. RY (1) C 44	0.07	1.79	0.010
135. BD (1) C 10- H 11	1022. RY (4) C 44	0.16	2.20	0.017
135. BD (1) C 10- H 11	1029. RY (11) C 44	0.09	3.00	0.015
136. BD (1) C 10- C 12	185. BD* (1) Pt 1- S 3	0.13	0.81	0.009
136. BD (1) C 10- C 12	252. RY (5) Pt 1	0.14	3.12	0.018
136. BD (1) C 10- C 12	255. RY (8) Pt 1	0.13	3.04	0.017
136. BD (1) C 10- C 12	257. RY (10) Pt 1	0.13	4.91	0.023
136. BD (1) C 10- C 12	258. RY (11) Pt 1	0.08	3.24	0.014
136. BD (1) C 10- C 12	259. RY (12) Pt 1	0.06	3.22	0.012
136. BD (1) C 10- C 12	260. RY (13) Pt 1	0.14	7.80	0.029
136. BD (1) C 10- C 12	262. RY (15) Pt 1	0.06	3.60	0.014
136. BD (1) C 10- C 12	263. RY (16) Pt 1	0.05	3.40	0.012
136. BD (1) C 10- C 12	267. RY (20) Pt 1	0.07	4.62	0.016
136. BD (1) C 10- C 12	273. RY (26) Pt 1	0.28	37.46	0.091
136. BD (1) C 10- C 12	276. RY (29) Pt 1	0.11	237.16	0.142
136. BD (1) C 10- C 12	281. RY (4) S 2	0.08	2.09	0.012
136. BD (1) C 10- C 12	282. RY (5) S 2	0.13	5.55	0.024
136. BD (1) C 10- C 12	283. RY (6) S 2	0.09	2.24	0.013
136. BD (1) C 10- C 12	309. RY (4) S 3	0.08	1.97	0.012
136. BD (1) C 10- C 12	310. RY (5) S 3	0.19	4.17	0.025
136. BD (1) C 10- C 12	311. RY (6) S 3	0.16	4.29	0.024
141. BD (1) C 14- C 16	260. RY (13) Pt 1	0.06	7.83	0.020
141. BD (1) C 14- C 16	273. RY (26) Pt 1	0.07	37.48	0.044
142. BD (1) C 16- C 17	185. BD* (1) Pt 1- S 3	0.31	0.79	0.014
142. BD (1) C 16- C 17	252. RY (5) Pt 1	0.06	3.10	0.012
142. BD (1) C 16- C 17	255. RY (8) Pt 1	0.09	3.02	0.014
142. BD (1) C 16- C 17	259. RY (12) Pt 1	0.08	3.20	0.015
142. BD (1) C 16- C 17	260. RY (13) Pt 1	0.07	7.78	0.021
142. BD (1) C 16- C 17	267. RY (20) Pt 1	0.14	4.60	0.023
142. BD (1) C 16- C 17	271. RY (24) Pt 1	0.13	5.33	0.023
142. BD (1) C 16- C 17	273. RY (26) Pt 1	0.13	37.44	0.063
142. BD (1) C 16- C 17	275. RY (28) Pt 1	0.06	28.26	0.038
142. BD (1) C 16- C 17	276. RY (29) Pt 1	0.08	237.14	0.122
142. BD (1) C 16- C 17	282. RY (5) S 2	0.07	5.53	0.017
142. BD (1) C 16- C 17	310. RY (5) S 3	0.08	4.15	0.016
142. BD (1) C 16- C 17	311. RY (6) S 3	0.08	4.27	0.016
144. BD (1) C 17- C 22	184. BD* (1) Pt 1- S 2	2.42	0.83	0.040
144. BD (1) C 17- C 22	185. BD* (1) Pt 1- S 3	2.42	0.84	0.040
144. BD (1) C 17- C 22	248. RY (1) Pt 1	1.60	2.61	0.058
144. BD (1) C 17- C 22	249. RY (2) Pt 1	2.55	3.20	0.081
144. BD (1) C 17- C 22	251. RY (4) Pt 1	0.07	2.69	0.012
144. BD (1) C 17- C 22	252. RY (5) Pt 1	1.87	3.15	0.068
144. BD (1) C 17- C 22	253. RY (6) Pt 1	0.45	3.61	0.036
144. BD (1) C 17- C 22	254. RY (7) Pt 1	0.05	2.47	0.010
144. BD (1) C 17- C 22	255. RY (8) Pt 1	2.15	3.07	0.073
144. BD (1) C 17- C 22	256. RY (9) Pt 1	0.96	3.16	0.049
144. BD (1) C 17- C 22	257. RY (10) Pt 1	2.85	4.94	0.106
144. BD (1) C 17- C 22	258. RY (11) Pt 1	0.78	3.27	0.045
144. BD (1) C 17- C 22	259. RY (12) Pt 1	1.03	3.25	0.052
144. BD (1) C 17- C 22	260. RY (13) Pt 1	2.93	7.84	0.135
144. BD (1) C 17- C 22	261. RY (14) Pt 1	0.23	2.80	0.023
144. BD (1) C 17- C 22	262. RY (15) Pt 1	2.04	3.63	0.077
144. BD (1) C 17- C 22	263. RY (16) Pt 1	1.21	3.44	0.057
144. BD (1) C 17- C 22	264. RY (17) Pt 1	0.12	2.93	0.017
144. BD (1) C 17- C 22	265. RY (18) Pt 1	0.90	4.16	0.055
144. BD (1) C 17- C 22	266. RY (19) Pt 1	1.05	4.14	0.059
144. BD (1) C 17- C 22	267. RY (20) Pt 1	1.96	4.65	0.085
144. BD (1) C 17- C 22	270. RY (23) Pt 1	0.10	2.63	0.015
144. BD (1) C 17- C 22	271. RY (24) Pt 1	2.32	5.39	0.100
144. BD (1) C 17- C 22	272. RY (25) Pt 1	0.09	2.77	0.014
144. BD (1) C 17- C 22	273. RY (26) Pt 1	4.44	37.49	0.364
144. BD (1) C 17- C 22	274. RY (27) Pt 1	0.44	27.74	0.099
144. BD (1) C 17- C 22	276. RY (29) Pt 1	1.95	237.19	0.607
144. BD (1) C 17- C 22	278. RY (1) S 2	0.05	1.57	0.008
144. BD (1) C 17- C 22	279. RY (2) S 2	0.72	1.86	0.033

144. BD (1) C 17- C 22	280. RY (3) S 2	0.17	1.55	0.015
144. BD (1) C 17- C 22	281. RY (4) S 2	1.31	2.12	0.047
144. BD (1) C 17- C 22	282. RY (5) S 2	3.29	5.58	0.121
144. BD (1) C 17- C 22	283. RY (6) S 2	1.47	2.27	0.052
144. BD (1) C 17- C 22	284. RY (7) S 2	0.43	2.35	0.028
144. BD (1) C 17- C 22	285. RY (8) S 2	0.51	2.46	0.032
144. BD (1) C 17- C 22	286. RY (9) S 2	0.47	2.75	0.032
144. BD (1) C 17- C 22	287. RY (10) S 2	0.14	2.56	0.017
144. BD (1) C 17- C 22	289. RY (12) S 2	0.20	3.60	0.024
144. BD (1) C 17- C 22	292. RY (15) S 2	0.06	2.80	0.012
144. BD (1) C 17- C 22	293. RY (16) S 2	0.31	3.54	0.029
144. BD (1) C 17- C 22	294. RY (17) S 2	0.23	3.65	0.026
144. BD (1) C 17- C 22	297. RY (20) S 2	0.39	4.10	0.036
144. BD (1) C 17- C 22	298. RY (21) S 2	0.06	3.38	0.012
144. BD (1) C 17- C 22	299. RY (22) S 2	0.83	4.96	0.057
144. BD (1) C 17- C 22	300. RY (23) S 2	0.08	3.14	0.014
144. BD (1) C 17- C 22	307. RY (2) S 3	0.42	1.59	0.023
144. BD (1) C 17- C 22	308. RY (3) S 3	0.22	1.60	0.017
144. BD (1) C 17- C 22	309. RY (4) S 3	1.16	2.00	0.043
144. BD (1) C 17- C 22	310. RY (5) S 3	2.84	4.20	0.098
144. BD (1) C 17- C 22	311. RY (6) S 3	3.11	4.32	0.103
144. BD (1) C 17- C 22	312. RY (7) S 3	0.58	2.52	0.034
144. BD (1) C 17- C 22	313. RY (8) S 3	0.14	2.29	0.016
144. BD (1) C 17- C 22	314. RY (9) S 3	0.20	2.55	0.020
144. BD (1) C 17- C 22	315. RY (10) S 3	0.21	2.60	0.021
144. BD (1) C 17- C 22	317. RY (12) S 3	0.22	3.60	0.025
144. BD (1) C 17- C 22	318. RY (13) S 3	0.06	2.88	0.011
144. BD (1) C 17- C 22	322. RY (17) S 3	0.40	4.10	0.036
144. BD (1) C 17- C 22	323. RY (18) S 3	0.32	3.66	0.031
144. BD (1) C 17- C 22	325. RY (20) S 3	0.62	4.14	0.045
144. BD (1) C 17- C 22	326. RY (21) S 3	0.14	3.59	0.020
144. BD (1) C 17- C 22	327. RY (22) S 3	0.68	3.53	0.044
144. BD (1) C 17- C 22	328. RY (23) S 3	0.11	3.19	0.016
144. BD (1) C 17- C 22	334. RY (1) S 4	0.42	1.65	0.024
144. BD (1) C 17- C 22	335. RY (2) S 4	0.09	1.68	0.011
144. BD (1) C 17- C 22	341. RY (8) S 4	0.17	2.18	0.017
144. BD (1) C 17- C 22	342. RY (9) S 4	0.07	2.31	0.011
144. BD (1) C 17- C 22	348. RY (15) S 4	0.15	2.92	0.019
144. BD (1) C 17- C 22	350. RY (17) S 4	0.15	3.34	0.020
144. BD (1) C 17- C 22	356. RY (23) S 4	0.05	3.94	0.013
144. BD (1) C 17- C 22	839. RY (1) C 29	0.11	2.03	0.013
144. BD (1) C 17- C 22	840. RY (2) C 29	0.60	1.79	0.029
144. BD (1) C 17- C 22	842. RY (4) C 29	0.37	2.34	0.026
144. BD (1) C 17- C 22	843. RY (5) C 29	0.30	2.52	0.025
144. BD (1) C 17- C 22	845. RY (7) C 29	0.05	1.95	0.009
144. BD (1) C 17- C 22	849. RY (11) C 29	0.12	2.70	0.016
144. BD (1) C 17- C 22	850. RY (12) C 29	0.19	3.68	0.023
144. BD (1) C 17- C 22	851. RY (13) C 29	0.09	3.44	0.016
144. BD (1) C 17- C 22	875. RY (1) C 32	0.47	1.97	0.027
144. BD (1) C 17- C 22	878. RY (4) C 32	0.43	2.40	0.029
144. BD (1) C 17- C 22	880. RY (6) C 32	0.12	2.12	0.014
144. BD (1) C 17- C 22	881. RY (7) C 32	0.11	2.26	0.014
144. BD (1) C 17- C 22	883. RY (9) C 32	0.06	3.27	0.012
144. BD (1) C 17- C 22	885. RY (11) C 32	0.23	2.89	0.023
144. BD (1) C 17- C 22	889. RY (15) C 32	0.11	4.50	0.020
144. BD (1) C 17- C 22	901. RY (1) H 33	0.05	2.17	0.009
144. BD (1) C 17- C 22	902. RY (2) H 33	0.07	2.76	0.013
144. BD (1) C 17- C 22	911. RY (1) C 35	0.51	1.92	0.028
144. BD (1) C 17- C 22	912. RY (2) C 35	0.17	2.43	0.018
144. BD (1) C 17- C 22	914. RY (4) C 35	0.67	2.41	0.036
144. BD (1) C 17- C 22	915. RY (5) C 35	0.16	2.42	0.018
144. BD (1) C 17- C 22	917. RY (7) C 35	0.07	2.32	0.011
144. BD (1) C 17- C 22	918. RY (8) C 35	0.13	2.61	0.017
144. BD (1) C 17- C 22	920. RY (10) C 35	0.07	2.70	0.012
144. BD (1) C 17- C 22	921. RY (11) C 35	0.17	2.93	0.020
144. BD (1) C 17- C 22	923. RY (13) C 35	0.21	4.31	0.027
144. BD (1) C 17- C 22	942. RY (1) H 37	0.07	1.94	0.010
144. BD (1) C 17- C 22	948. RY (2) C 38	0.09	2.19	0.013
144. BD (1) C 17- C 22	952. RY (6) C 38	0.27	2.24	0.022
144. BD (1) C 17- C 22	959. RY (13) C 38	0.15	3.07	0.019
144. BD (1) C 17- C 22	973. RY (1) H 39	0.26	1.94	0.020
144. BD (1) C 17- C 22	975. RY (3) H 39	0.10	3.17	0.016
144. BD (1) C 17- C 22	988. RY (6) C 41	0.16	2.61	0.018
144. BD (1) C 17- C 22	989. RY (7) C 41	0.06	2.17	0.010
144. BD (1) C 17- C 22	991. RY (9) C 41	0.08	3.06	0.014
144. BD (1) C 17- C 22	993. RY (11) C 41	0.07	3.33	0.013
144. BD (1) C 17- C 22	1019. RY (1) C 44	0.20	1.91	0.017
144. BD (1) C 17- C 22	1020. RY (2) C 44	0.12	2.30	0.015
144. BD (1) C 17- C 22	1022. RY (4) C 44	0.63	2.32	0.034
144. BD (1) C 17- C 22	1024. RY (6) C 44	0.12	2.37	0.015
144. BD (1) C 17- C 22	1027. RY (9) C 44	0.14	2.90	0.018
144. BD (1) C 17- C 22	1029. RY (11) C 44	0.33	3.11	0.029
144. BD (1) C 17- C 22	1031. RY (13) C 44	0.12	4.91	0.021
144. BD (1) C 17- C 22	1045. RY (1) H 45	0.19	1.98	0.017
144. BD (1) C 17- C 22	1050. RY (1) H 46	0.11	1.88	0.013
149. BD (1) C 21- C 22	184. BD* (1) Pt 1- S 2	0.17	0.81	0.010
149. BD (1) C 21- C 22	248. RY (1) Pt 1	0.08	2.59	0.013
149. BD (1) C 21- C 22	249. RY (2) Pt 1	0.08	3.18	0.015
149. BD (1) C 21- C 22	252. RY (5) Pt 1	0.10	3.13	0.016
149. BD (1) C 21- C 22	255. RY (8) Pt 1	0.15	3.05	0.019
149. BD (1) C 21- C 22	257. RY (10) Pt 1	0.17	4.92	0.026
149. BD (1) C 21- C 22	258. RY (11) Pt 1	0.12	3.24	0.017
149. BD (1) C 21- C 22	259. RY (12) Pt 1	0.10	3.22	0.016
149. BD (1) C 21- C 22	260. RY (13) Pt 1	0.20	7.81	0.035
149. BD (1) C 21- C 22	262. RY (15) Pt 1	0.13	3.61	0.019
149. BD (1) C 21- C 22	263. RY (16) Pt 1	0.09	3.41	0.015
149. BD (1) C 21- C 22	266. RY (19) Pt 1	0.20	4.11	0.026
149. BD (1) C 21- C 22	267. RY (20) Pt 1	0.05	4.62	0.014
149. BD (1) C 21- C 22	271. RY (24) Pt 1	0.22	5.36	0.031
149. BD (1) C 21- C 22	273. RY (26) Pt 1	0.29	37.46	0.093
149. BD (1) C 21- C 22	276. RY (29) Pt 1	0.16	237.16	0.175
149. BD (1) C 21- C 22	279. RY (2) S 2	0.07	1.84	0.010
149. BD (1) C 21- C 22	281. RY (4) S 2	0.05	2.10	0.010

149. BD (1) C 21- C 22	282. RY (5) S 2	0.19	5.55	0.029
149. BD (1) C 21- C 22	283. RY (6) S 2	0.08	2.25	0.012
149. BD (1) C 21- C 22	309. RY (4) S 3	0.05	1.98	0.009
149. BD (1) C 21- C 22	310. RY (5) S 3	0.13	4.18	0.021
149. BD (1) C 21- C 22	311. RY (6) S 3	0.14	4.30	0.022
150. BD (2) C 21- C 22	257. RY (10)Pt 1	0.08	4.47	0.017
150. BD (2) C 21- C 22	260. RY (13)Pt 1	0.07	7.37	0.021
150. BD (2) C 21- C 22	273. RY (26)Pt 1	0.12	37.02	0.059
150. BD (2) C 21- C 22	282. RY (5) S 2	0.08	5.11	0.018
150. BD (2) C 21- C 22	310. RY (5) S 3	0.08	3.73	0.016
150. BD (2) C 21- C 22	311. RY (6) S 3	0.08	3.85	0.016
151. BD (1) C 21- C 23	255. RY (8)Pt 1	0.05	3.07	0.011
151. BD (1) C 21- C 23	257. RY (10)Pt 1	0.08	4.94	0.018
151. BD (1) C 21- C 23	260. RY (13)Pt 1	0.09	7.83	0.023
151. BD (1) C 21- C 23	271. RY (24)Pt 1	0.05	5.38	0.015
151. BD (1) C 21- C 23	273. RY (26)Pt 1	0.07	37.48	0.047
151. BD (1) C 21- C 23	276. RY (29)Pt 1	0.05	237.18	0.099
151. BD (1) C 21- C 23	282. RY (5) S 2	0.05	5.57	0.015
156. BD (1) C 25- C 27	184. BD* (1)Pt 1- S 2	0.19	0.78	0.011
156. BD (1) C 25- C 27	252. RY (5)Pt 1	0.10	3.10	0.015
156. BD (1) C 25- C 27	255. RY (8)Pt 1	0.09	3.02	0.015
156. BD (1) C 25- C 27	256. RY (9)Pt 1	0.06	3.10	0.012
156. BD (1) C 25- C 27	257. RY (10)Pt 1	0.08	4.88	0.018
156. BD (1) C 25- C 27	258. RY (11)Pt 1	0.05	3.21	0.012
156. BD (1) C 25- C 27	259. RY (12)Pt 1	0.09	3.19	0.015
156. BD (1) C 25- C 27	260. RY (13)Pt 1	0.16	7.78	0.032
156. BD (1) C 25- C 27	262. RY (15)Pt 1	0.08	3.58	0.015
156. BD (1) C 25- C 27	263. RY (16)Pt 1	0.05	3.38	0.012
156. BD (1) C 25- C 27	266. RY (19)Pt 1	0.07	4.08	0.015
156. BD (1) C 25- C 27	273. RY (26)Pt 1	0.25	37.43	0.087
156. BD (1) C 25- C 27	276. RY (29)Pt 1	0.11	237.13	0.143
156. BD (1) C 25- C 27	281. RY (4) S 2	0.06	2.06	0.010
156. BD (1) C 25- C 27	282. RY (5) S 2	0.18	5.52	0.028
156. BD (1) C 25- C 27	283. RY (6) S 2	0.06	2.22	0.010
156. BD (1) C 25- C 27	310. RY (5) S 3	0.09	4.14	0.018
156. BD (1) C 25- C 27	311. RY (6) S 3	0.15	4.26	0.023
157. BD (1) C 27- H 28	184. BD* (1)Pt 1- S 2	0.85	0.71	0.022
157. BD (1) C 27- H 28	185. BD* (1)Pt 1- S 3	0.71	0.72	0.020
157. BD (1) C 27- H 28	188. BD* (1) S 3- C 32	0.05	0.66	0.005
157. BD (1) C 27- H 28	248. RY (1)Pt 1	0.47	2.49	0.031
157. BD (1) C 27- H 28	249. RY (2)Pt 1	0.30	3.08	0.027
157. BD (1) C 27- H 28	252. RY (5)Pt 1	0.42	3.03	0.032
157. BD (1) C 27- H 28	253. RY (6)Pt 1	0.20	3.49	0.023
157. BD (1) C 27- H 28	255. RY (8)Pt 1	0.38	2.96	0.030
157. BD (1) C 27- H 28	256. RY (9)Pt 1	0.33	3.04	0.028
157. BD (1) C 27- H 28	257. RY (10)Pt 1	0.73	4.82	0.053
157. BD (1) C 27- H 28	258. RY (11)Pt 1	0.14	3.15	0.019
157. BD (1) C 27- H 28	259. RY (12)Pt 1	0.16	3.13	0.020
157. BD (1) C 27- H 28	260. RY (13)Pt 1	0.67	7.72	0.064
157. BD (1) C 27- H 28	262. RY (15)Pt 1	0.67	3.51	0.043
157. BD (1) C 27- H 28	263. RY (16)Pt 1	0.34	3.32	0.030
157. BD (1) C 27- H 28	265. RY (18)Pt 1	0.26	4.04	0.029
157. BD (1) C 27- H 28	266. RY (19)Pt 1	0.44	4.02	0.038
157. BD (1) C 27- H 28	267. RY (20)Pt 1	0.26	4.53	0.031
157. BD (1) C 27- H 28	271. RY (24)Pt 1	0.37	5.27	0.040
157. BD (1) C 27- H 28	272. RY (25)Pt 1	0.09	2.66	0.014
157. BD (1) C 27- H 28	273. RY (26)Pt 1	1.11	37.37	0.182
157. BD (1) C 27- H 28	276. RY (29)Pt 1	0.35	237.07	0.259
157. BD (1) C 27- H 28	279. RY (2) S 2	0.20	1.74	0.017
157. BD (1) C 27- H 28	280. RY (3) S 2	0.06	1.43	0.008
157. BD (1) C 27- H 28	281. RY (4) S 2	0.39	2.00	0.025
157. BD (1) C 27- H 28	282. RY (5) S 2	0.94	5.46	0.064
157. BD (1) C 27- H 28	283. RY (6) S 2	0.47	2.15	0.028
157. BD (1) C 27- H 28	284. RY (7) S 2	0.13	2.23	0.015
157. BD (1) C 27- H 28	285. RY (8) S 2	0.13	2.34	0.015
157. BD (1) C 27- H 28	286. RY (9) S 2	0.15	2.63	0.018
157. BD (1) C 27- H 28	289. RY (12) S 2	0.05	3.49	0.012
157. BD (1) C 27- H 28	293. RY (16) S 2	0.08	3.42	0.014
157. BD (1) C 27- H 28	294. RY (17) S 2	0.06	3.53	0.013
157. BD (1) C 27- H 28	297. RY (20) S 2	0.09	3.98	0.016
157. BD (1) C 27- H 28	299. RY (22) S 2	0.20	4.84	0.027
157. BD (1) C 27- H 28	307. RY (2) S 3	0.10	1.47	0.011
157. BD (1) C 27- H 28	308. RY (3) S 3	0.05	1.48	0.008
157. BD (1) C 27- H 28	309. RY (4) S 3	0.18	1.88	0.017
157. BD (1) C 27- H 28	310. RY (5) S 3	0.59	4.08	0.044
157. BD (1) C 27- H 28	311. RY (6) S 3	1.03	4.20	0.059
157. BD (1) C 27- H 28	312. RY (7) S 3	0.17	2.41	0.018
157. BD (1) C 27- H 28	313. RY (8) S 3	0.05	2.17	0.010
157. BD (1) C 27- H 28	315. RY (10) S 3	0.11	2.48	0.015
157. BD (1) C 27- H 28	317. RY (12) S 3	0.17	3.48	0.022
157. BD (1) C 27- H 28	322. RY (17) S 3	0.16	3.98	0.023
157. BD (1) C 27- H 28	323. RY (18) S 3	0.12	3.54	0.018
157. BD (1) C 27- H 28	325. RY (20) S 3	0.23	4.02	0.027
157. BD (1) C 27- H 28	327. RY (22) S 3	0.21	3.41	0.024
157. BD (1) C 27- H 28	334. RY (1) S 4	0.12	1.53	0.012
157. BD (1) C 27- H 28	840. RY (2) C 29	0.16	1.67	0.015
157. BD (1) C 27- H 28	842. RY (4) C 29	0.09	2.22	0.013
157. BD (1) C 27- H 28	843. RY (5) C 29	0.08	2.40	0.012
157. BD (1) C 27- H 28	875. RY (1) C 32	0.11	1.85	0.013
157. BD (1) C 27- H 28	878. RY (4) C 32	0.11	2.29	0.014
157. BD (1) C 27- H 28	885. RY (11) C 32	0.06	2.77	0.012
157. BD (1) C 27- H 28	911. RY (1) C 35	0.15	1.80	0.015
157. BD (1) C 27- H 28	912. RY (2) C 35	0.06	2.31	0.010
157. BD (1) C 27- H 28	914. RY (4) C 35	0.19	2.29	0.019
157. BD (1) C 27- H 28	923. RY (13) C 35	0.06	4.19	0.014
157. BD (1) C 27- H 28	952. RY (6) C 38	0.06	2.12	0.010
157. BD (1) C 27- H 28	973. RY (1) H 39	0.05	1.82	0.009
157. BD (1) C 27- H 28	988. RY (6) C 41	0.05	2.50	0.010
157. BD (1) C 27- H 28	1019. RY (1) C 44	0.08	1.79	0.010
157. BD (1) C 27- H 28	1022. RY (4) C 44	0.16	2.20	0.017
157. BD (1) C 27- H 28	1029. RY (11) C 44	0.08	2.99	0.014

from unit 2 to unit 3						
92. LP (1) N 7	1064. RY (10)Sb 47	0.18	2.53	0.019		
92. LP (1) N 7	1066. RY (12)Sb 47	0.53	1.84	0.028		
92. LP (1) N 7	1067. RY (13)Sb 47	0.65	1.83	0.031		
92. LP (1) N 7	1070. RY (16)Sb 47	0.88	5.17	0.060		
92. LP (1) N 7	1071. RY (17)Sb 47	0.27	2.26	0.022		
92. LP (1) N 7	1075. RY (21)Sb 47	0.08	3.12	0.014		
92. LP (1) N 7	1076. RY (22)Sb 47	0.12	10.31	0.031		
92. LP (1) N 7	1083. RY (29)Sb 47	0.05	34.02	0.038		
92. LP (1) N 7	1181. RY (6)Cl 51	0.11	2.01	0.013		
93. LP (1) N 8	1064. RY (10)Sb 47	0.23	2.53	0.021		
93. LP (1) N 8	1065. RY (11)Sb 47	0.06	2.78	0.012		
93. LP (1) N 8	1066. RY (12)Sb 47	0.50	1.84	0.027		
93. LP (1) N 8	1067. RY (13)Sb 47	0.78	1.82	0.034		
93. LP (1) N 8	1069. RY (15)Sb 47	0.08	1.68	0.010		
93. LP (1) N 8	1070. RY (16)Sb 47	0.94	5.16	0.062		
93. LP (1) N 8	1071. RY (17)Sb 47	0.38	2.26	0.026		
93. LP (1) N 8	1075. RY (21)Sb 47	0.07	3.12	0.013		
93. LP (1) N 8	1076. RY (22)Sb 47	0.13	10.30	0.033		
93. LP (1) N 8	1083. RY (29)Sb 47	0.06	34.02	0.041		
93. LP (1) N 8	1085. RY (31)Sb 47	0.06	2.21	0.010		
93. LP (1) N 8	1176. RY (1)Cl 51	0.05	1.86	0.009		
93. LP (1) N 8	1181. RY (6)Cl 51	0.11	2.01	0.013		
129. BD (2) N 7- C 10	1059. RY (5)Sb 47	0.11	1.69	0.012		
133. BD (2) N 8- C 27	1060. RY (6)Sb 47	0.08	1.22	0.009		
135. BD (1) C 10- H 11	1067. RY (13)Sb 47	0.07	1.94	0.010		
135. BD (1) C 10- H 11	1070. RY (16)Sb 47	0.09	5.28	0.019		
142. BD (1) C 16- C 17	240. BD* (1)Sb 47-Cl 51	0.06	0.80	0.006		
144. BD (1) C 17- C 22	1064. RY (10)Sb 47	0.06	2.76	0.011		
144. BD (1) C 17- C 22	1066. RY (12)Sb 47	0.15	2.07	0.016		
144. BD (1) C 17- C 22	1067. RY (13)Sb 47	0.20	2.05	0.018		
144. BD (1) C 17- C 22	1070. RY (16)Sb 47	0.37	5.39	0.040		
144. BD (1) C 17- C 22	1071. RY (17)Sb 47	0.10	2.49	0.014		
144. BD (1) C 17- C 22	1076. RY (22)Sb 47	0.06	10.53	0.022		
149. BD (1) C 21- C 22	240. BD* (1)Sb 47-Cl 51	0.07	0.83	0.007		
157. BD (1) C 27- H 28	1067. RY (13)Sb 47	0.06	1.93	0.010		
157. BD (1) C 27- H 28	1070. RY (16)Sb 47	0.08	5.27	0.018		
from unit 2 to unit 4						
92. LP (1) N 7	1092. RY (1)Cl 48	0.13	1.30	0.012		
92. LP (1) N 7	1093. RY (2)Cl 48	0.11	1.72	0.013		
92. LP (1) N 7	1098. RY (7)Cl 48	0.25	2.12	0.021		
92. LP (1) N 7	1100. RY (9)Cl 48	0.14	1.51	0.013		
93. LP (1) N 8	1092. RY (1)Cl 48	0.14	1.29	0.012		
93. LP (1) N 8	1093. RY (2)Cl 48	0.07	1.72	0.010		
93. LP (1) N 8	1098. RY (7)Cl 48	0.20	2.12	0.019		
93. LP (1) N 8	1100. RY (9)Cl 48	0.15	1.51	0.013		
144. BD (1) C 17- C 22	1098. RY (7)Cl 48	0.08	2.35	0.012		
from unit 2 to unit 5						
92. LP (1) N 7	1124. RY (5)Cl 49	0.07	2.34	0.012		
92. LP (1) N 7	1127. RY (8)Cl 49	0.06	2.99	0.012		
93. LP (1) N 8	1124. RY (5)Cl 49	0.09	2.33	0.013		
from unit 2 to unit 6						
92. LP (1) N 7	1148. RY (1)Cl 50	0.12	1.32	0.011		
92. LP (1) N 7	1153. RY (6)Cl 50	0.26	1.73	0.019		
92. LP (1) N 7	1154. RY (7)Cl 50	0.27	1.81	0.020		
92. LP (1) N 7	1155. RY (8)Cl 50	0.28	2.73	0.025		
92. LP (1) N 7	1156. RY (9)Cl 50	0.18	1.89	0.016		
93. LP (1) N 8	1148. RY (1)Cl 50	0.11	1.32	0.011		
93. LP (1) N 8	1153. RY (6)Cl 50	0.22	1.72	0.017		
93. LP (1) N 8	1154. RY (7)Cl 50	0.35	1.81	0.022		
93. LP (1) N 8	1155. RY (8)Cl 50	0.38	2.73	0.029		
93. LP (1) N 8	1156. RY (9)Cl 50	0.15	1.88	0.015		
144. BD (1) C 17- C 22	1153. RY (6)Cl 50	0.08	1.95	0.011		
144. BD (1) C 17- C 22	1154. RY (7)Cl 50	0.08	2.04	0.012		
144. BD (1) C 17- C 22	1155. RY (8)Cl 50	0.11	2.96	0.016		
144. BD (1) C 17- C 22	1156. RY (9)Cl 50	0.07	2.11	0.011		
from unit 2 to unit 7						
92. LP (1) N 7	1204. RY (1)Cl 52	0.11	1.35	0.011		
92. LP (1) N 7	1205. RY (2)Cl 52	0.28	2.03	0.021		
93. LP (1) N 8	1204. RY (1)Cl 52	0.15	1.34	0.013		
93. LP (1) N 8	1205. RY (2)Cl 52	0.41	2.02	0.026		
93. LP (1) N 8	1208. RY (5)Cl 52	0.07	2.77	0.013		
93. LP (1) N 8	1210. RY (7)Cl 52	0.07	2.46	0.012		
144. BD (1) C 17- C 22	1205. RY (2)Cl 52	0.13	2.25	0.015		
from unit 2 to unit 8						
None above threshold						
from unit 3 to unit 1						
43. CR (1)Sb 47	248. RY (1)Pt 1	0.23	8.28	0.039		
43. CR (1)Sb 47	252. RY (5)Pt 1	0.22	8.82	0.039		
47. CR (5)Sb 47	252. RY (5)Pt 1	0.10	4.19	0.018		
68. CR (2)Cl 51	248. RY (1)Pt 1	0.06	16.33	0.028		
68. CR (2)Cl 51	252. RY (5)Pt 1	0.05	16.87	0.026		
96. LP (1)Sb 47	249. RY (2)Pt 1	0.15	2.83	0.018		
96. LP (1)Sb 47	251. RY (4)Pt 1	0.26	2.31	0.022		
96. LP (1)Sb 47	254. RY (7)Pt 1	0.41	2.10	0.026		
96. LP (1)Sb 47	257. RY (10)Pt 1	0.15	4.57	0.024		
96. LP (1)Sb 47	258. RY (11)Pt 1	0.09	2.90	0.015		
96. LP (1)Sb 47	262. RY (15)Pt 1	0.06	3.26	0.012		
96. LP (1)Sb 47	263. RY (16)Pt 1	0.21	3.07	0.022		
96. LP (1)Sb 47	265. RY (18)Pt 1	0.11	3.79	0.018		
96. LP (1)Sb 47	267. RY (20)Pt 1	0.11	4.28	0.019		
96. LP (1)Sb 47	269. RY (22)Pt 1	0.11	2.37	0.014		
96. LP (1)Sb 47	271. RY (24)Pt 1	0.14	5.02	0.023		
96. LP (1)Sb 47	273. RY (26)Pt 1	0.30	37.12	0.095		
96. LP (1)Sb 47	277. RY (30)Pt 1	0.13	27.45	0.053		
96. LP (1)Sb 47	281. RY (4) S 2	0.16	1.75	0.015		
96. LP (1)Sb 47	282. RY (5) S 2	0.36	5.21	0.038		

96. LP (1)Sb 47	283. RY (6) S 2	0.29	1.90	0.021
96. LP (1)Sb 47	286. RY (9) S 2	0.09	2.38	0.013
96. LP (1)Sb 47	297. RY (20) S 2	0.07	3.73	0.014
96. LP (1)Sb 47	309. RY (4) S 3	0.12	1.63	0.013
96. LP (1)Sb 47	310. RY (5) S 3	0.37	3.83	0.034
96. LP (1)Sb 47	311. RY (6) S 3	0.41	3.95	0.036
96. LP (1)Sb 47	315. RY (10) S 3	0.05	2.23	0.010
96. LP (1)Sb 47	325. RY (20) S 3	0.05	3.77	0.012
96. LP (1)Sb 47	327. RY (22) S 3	0.08	3.16	0.015
96. LP (1)Sb 47	334. RY (1) S 4	0.11	1.28	0.010
96. LP (1)Sb 47	341. RY (8) S 4	0.09	1.81	0.011
96. LP (1)Sb 47	840. RY (2) C 29	0.05	1.42	0.008
96. LP (1)Sb 47	842. RY (4) C 29	0.13	1.97	0.014
96. LP (1)Sb 47	875. RY (1) C 32	0.09	1.60	0.011
96. LP (1)Sb 47	878. RY (4) C 32	0.09	2.03	0.012
96. LP (1)Sb 47	952. RY (6) C 38	0.07	1.87	0.010
96. LP (1)Sb 47	1022. RY (4) C 44	0.06	1.95	0.009
109. LP (1)Cl 51	184. BD* (1)Pt 1- S 2	0.12	0.79	0.009
109. LP (1)Cl 51	185. BD* (1)Pt 1- S 3	0.12	0.79	0.009
109. LP (1)Cl 51	252. RY (5)Pt 1	0.18	3.11	0.021
109. LP (1)Cl 51	255. RY (8)Pt 1	0.06	3.03	0.012
109. LP (1)Cl 51	256. RY (9)Pt 1	0.07	3.11	0.013
109. LP (1)Cl 51	257. RY (10)Pt 1	0.13	4.90	0.023
109. LP (1)Cl 51	260. RY (13)Pt 1	0.08	7.79	0.023
109. LP (1)Cl 51	262. RY (15)Pt 1	0.08	3.59	0.015
109. LP (1)Cl 51	267. RY (20)Pt 1	0.06	4.60	0.015
109. LP (1)Cl 51	271. RY (24)Pt 1	0.06	5.34	0.016
109. LP (1)Cl 51	273. RY (26)Pt 1	0.12	37.44	0.060
109. LP (1)Cl 51	281. RY (4) S 2	0.06	2.07	0.010
109. LP (1)Cl 51	282. RY (5) S 2	0.13	5.53	0.024
109. LP (1)Cl 51	283. RY (6) S 2	0.07	2.23	0.011
109. LP (1)Cl 51	310. RY (5) S 3	0.10	4.16	0.018
109. LP (1)Cl 51	311. RY (6) S 3	0.14	4.28	0.022
173. BD (1)Sb 47-cl 51	248. RY (1)Pt 1	2.32	2.30	0.065
173. BD (1)Sb 47-cl 51	252. RY (5)Pt 1	0.20	2.84	0.021
173. BD (1)Sb 47-cl 51	253. RY (6)Pt 1	0.15	3.29	0.020
173. BD (1)Sb 47-cl 51	254. RY (7)Pt 1	0.15	2.15	0.016
173. BD (1)Sb 47-cl 51	255. RY (8)Pt 1	0.23	2.76	0.022
173. BD (1)Sb 47-cl 51	256. RY (9)Pt 1	0.13	2.84	0.017
173. BD (1)Sb 47-cl 51	257. RY (10)Pt 1	0.20	4.63	0.027
173. BD (1)Sb 47-cl 51	260. RY (13)Pt 1	0.29	7.52	0.042
173. BD (1)Sb 47-cl 51	262. RY (15)Pt 1	0.10	3.32	0.016
173. BD (1)Sb 47-cl 51	263. RY (16)Pt 1	0.16	3.12	0.020
173. BD (1)Sb 47-cl 51	266. RY (19)Pt 1	0.06	3.82	0.014
173. BD (1)Sb 47-cl 51	267. RY (20)Pt 1	0.08	4.33	0.017
173. BD (1)Sb 47-cl 51	271. RY (24)Pt 1	0.07	5.07	0.017
173. BD (1)Sb 47-cl 51	272. RY (25)Pt 1	0.05	2.46	0.010
173. BD (1)Sb 47-cl 51	273. RY (26)Pt 1	0.27	37.17	0.090
173. BD (1)Sb 47-cl 51	276. RY (29)Pt 1	0.07	236.87	0.112
173. BD (1)Sb 47-cl 51	279. RY (2) S 2	0.07	1.55	0.009
173. BD (1)Sb 47-cl 51	281. RY (4) S 2	0.12	1.81	0.013
173. BD (1)Sb 47-cl 51	282. RY (5) S 2	0.29	5.26	0.035
173. BD (1)Sb 47-cl 51	283. RY (6) S 2	0.13	1.96	0.014
173. BD (1)Sb 47-cl 51	299. RY (22) S 2	0.06	4.64	0.015
173. BD (1)Sb 47-cl 51	309. RY (4) S 3	0.10	1.69	0.012
173. BD (1)Sb 47-cl 51	310. RY (5) S 3	0.22	3.89	0.026
173. BD (1)Sb 47-cl 51	311. RY (6) S 3	0.27	4.01	0.029
173. BD (1)Sb 47-cl 51	322. RY (17) S 3	0.05	3.79	0.013
173. BD (1)Sb 47-cl 51	325. RY (20) S 3	0.05	3.83	0.013
173. BD (1)Sb 47-cl 51	840. RY (2) C 29	0.06	1.47	0.008
173. BD (1)Sb 47-cl 51	911. RY (1) C 35	0.05	1.60	0.008
173. BD (1)Sb 47-cl 51	914. RY (4) C 35	0.09	2.09	0.012
173. BD (1)Sb 47-cl 51	1022. RY (4) C 44	0.06	2.00	0.009
from unit 3 to unit 2				
96. LP (1)Sb 47	196. BD* (2) N 7- C 10	0.05	0.27	0.003
96. LP (1)Sb 47	414. RY (1) N 7	0.27	4.77	0.032
96. LP (1)Sb 47	415. RY (2) N 7	0.17	1.30	0.013
96. LP (1)Sb 47	416. RY (3) N 7	0.11	1.81	0.013
96. LP (1)Sb 47	426. RY (13) N 7	0.05	4.34	0.013
96. LP (1)Sb 47	440. RY (1) N 8	0.28	4.70	0.032
96. LP (1)Sb 47	441. RY (2) N 8	0.18	1.44	0.014
96. LP (1)Sb 47	442. RY (3) N 8	0.07	1.79	0.010
96. LP (1)Sb 47	452. RY (13) N 8	0.09	3.84	0.016
96. LP (1)Sb 47	611. RY (1) C 17	0.15	2.59	0.017
96. LP (1)Sb 47	613. RY (3) C 17	0.13	1.52	0.013
96. LP (1)Sb 47	614. RY (4) C 17	0.17	2.89	0.020
96. LP (1)Sb 47	615. RY (5) C 17	0.11	3.27	0.017
96. LP (1)Sb 47	616. RY (6) C 17	0.08	2.66	0.013
96. LP (1)Sb 47	622. RY (12) C 17	0.14	3.55	0.020
96. LP (1)Sb 47	720. RY (1) C 22	0.10	2.43	0.014
96. LP (1)Sb 47	721. RY (2) C 22	0.06	1.99	0.010
96. LP (1)Sb 47	722. RY (3) C 22	0.09	1.66	0.011
96. LP (1)Sb 47	723. RY (4) C 22	0.15	2.78	0.018
96. LP (1)Sb 47	724. RY (5) C 22	0.05	2.77	0.011
96. LP (1)Sb 47	730. RY (11) C 22	0.17	3.83	0.023
96. LP (1)Sb 47	808. RY (1) C 27	0.08	2.23	0.012
96. LP (1)Sb 47	834. RY (1) H 28	0.16	1.96	0.016
109. LP (1)Cl 51	414. RY (1) N 7	0.15	5.09	0.025
109. LP (1)Cl 51	440. RY (1) N 8	0.15	5.03	0.025
109. LP (1)Cl 51	614. RY (4) C 17	0.06	3.22	0.013
109. LP (1)Cl 51	723. RY (4) C 22	0.06	3.11	0.012
109. LP (1)Cl 51	834. RY (1) H 28	0.05	2.28	0.010
173. BD (1)Sb 47-cl 51	414. RY (1) N 7	0.27	4.82	0.032
173. BD (1)Sb 47-cl 51	415. RY (2) N 7	0.16	1.36	0.013
173. BD (1)Sb 47-cl 51	440. RY (1) N 8	0.29	4.76	0.033
173. BD (1)Sb 47-cl 51	441. RY (2) N 8	0.19	1.50	0.015
173. BD (1)Sb 47-cl 51	452. RY (13) N 8	0.05	3.90	0.013
173. BD (1)Sb 47-cl 51	495. RY (4) C 10	0.09	1.89	0.012
173. BD (1)Sb 47-cl 51	499. RY (8) C 10	0.08	3.08	0.014
173. BD (1)Sb 47-cl 51	611. RY (1) C 17	0.08	2.64	0.013
173. BD (1)Sb 47-cl 51	614. RY (4) C 17	0.10	2.95	0.015
173. BD (1)Sb 47-cl 51	720. RY (1) C 22	0.09	2.48	0.013

173. BD (1)Sb 47-C1 51	723. RY (4) C 22	0.13	2.84	0.017
173. BD (1)Sb 47-C1 51	808. RY (1) C 27	0.06	2.28	0.010
173. BD (1)Sb 47-C1 51	811. RY (4) C 27	0.08	2.06	0.011
173. BD (1)Sb 47-C1 51	813. RY (6) C 27	0.05	2.42	0.010
173. BD (1)Sb 47-C1 51	815. RY (8) C 27	0.05	3.49	0.012
173. BD (1)Sb 47-C1 51	834. RY (1) H 28	0.09	2.01	0.012
within unit 3				
44. CR (2)Sb 47	183. LV (2)Sb 47	1.32	4.64	0.070
44. CR (2)Sb 47	240. BD* (1)Sb 47-C1 51	1.20	4.69	0.067
44. CR (2)Sb 47	1055. RY (1)Sb 47	1.13	5.47	0.070
44. CR (2)Sb 47	1057. RY (3)Sb 47	0.55	5.29	0.048
44. CR (2)Sb 47	1058. RY (4)Sb 47	0.64	5.22	0.051
44. CR (2)Sb 47	1071. RY (17)Sb 47	0.93	6.32	0.069
45. CR (3)Sb 47	183. LV (2)Sb 47	1.64	4.64	0.078
45. CR (3)Sb 47	240. BD* (1)Sb 47-C1 51	0.76	4.69	0.053
45. CR (3)Sb 47	1055. RY (1)Sb 47	0.65	5.47	0.053
45. CR (3)Sb 47	1057. RY (3)Sb 47	1.41	5.29	0.077
45. CR (3)Sb 47	1072. RY (18)Sb 47	0.79	6.43	0.064
46. CR (4)Sb 47	182. LV (1)Sb 47	2.66	4.64	0.099
46. CR (4)Sb 47	1058. RY (4)Sb 47	2.32	5.22	0.098
47. CR (5)Sb 47	1055. RY (1)Sb 47	5.15	2.67	0.105
47. CR (5)Sb 47	1056. RY (2)Sb 47	4.08	2.59	0.092
47. CR (5)Sb 47	1057. RY (3)Sb 47	0.51	2.50	0.032
47. CR (5)Sb 47	1061. RY (7)Sb 47	3.72	3.02	0.095
47. CR (5)Sb 47	1062. RY (8)Sb 47	2.40	2.46	0.068
47. CR (5)Sb 47	1066. RY (12)Sb 47	0.89	3.10	0.047
47. CR (5)Sb 47	1067. RY (13)Sb 47	0.96	3.09	0.048
47. CR (5)Sb 47	1070. RY (16)Sb 47	1.84	6.43	0.097
47. CR (5)Sb 47	1074. RY (20)Sb 47	0.94	3.70	0.052
47. CR (5)Sb 47	1085. RY (31)Sb 47	0.59	3.47	0.040
48. CR (6)Sb 47	1055. RY (1)Sb 47	0.94	2.67	0.045
48. CR (6)Sb 47	1056. RY (2)Sb 47	3.02	2.59	0.079
48. CR (6)Sb 47	1057. RY (3)Sb 47	0.65	2.50	0.036
48. CR (6)Sb 47	1059. RY (5)Sb 47	3.30	3.06	0.090
48. CR (6)Sb 47	1060. RY (6)Sb 47	0.52	2.58	0.033
48. CR (6)Sb 47	1061. RY (7)Sb 47	0.55	3.02	0.036
48. CR (6)Sb 47	1062. RY (8)Sb 47	5.12	2.46	0.100
48. CR (6)Sb 47	1074. RY (20)Sb 47	3.12	3.70	0.096
48. CR (6)Sb 47	1075. RY (21)Sb 47	1.99	4.38	0.083
48. CR (6)Sb 47	1082. RY (28)Sb 47	0.56	3.98	0.042
48. CR (6)Sb 47	1085. RY (31)Sb 47	2.89	3.47	0.089
49. CR (7)Sb 47	1055. RY (1)Sb 47	0.99	2.67	0.046
49. CR (7)Sb 47	1059. RY (5)Sb 47	3.82	3.06	0.097
49. CR (7)Sb 47	1060. RY (6)Sb 47	1.46	2.58	0.055
49. CR (7)Sb 47	1062. RY (8)Sb 47	5.95	2.46	0.108
49. CR (7)Sb 47	1073. RY (19)Sb 47	0.60	3.90	0.043
49. CR (7)Sb 47	1074. RY (20)Sb 47	3.22	3.70	0.097
49. CR (7)Sb 47	1079. RY (25)Sb 47	2.55	4.33	0.094
49. CR (7)Sb 47	1082. RY (28)Sb 47	0.50	3.98	0.040
49. CR (7)Sb 47	1085. RY (31)Sb 47	3.76	3.47	0.102
50. CR (8)Sb 47	1057. RY (3)Sb 47	1.00	2.49	0.045
50. CR (8)Sb 47	1059. RY (5)Sb 47	1.38	3.06	0.058
50. CR (8)Sb 47	1060. RY (6)Sb 47	6.80	2.58	0.118
50. CR (8)Sb 47	1061. RY (7)Sb 47	1.58	3.02	0.062
50. CR (8)Sb 47	1069. RY (15)Sb 47	0.70	2.94	0.040
50. CR (8)Sb 47	1074. RY (20)Sb 47	3.82	3.70	0.106
50. CR (8)Sb 47	1075. RY (21)Sb 47	4.46	4.38	0.125
50. CR (8)Sb 47	1082. RY (28)Sb 47	1.57	3.98	0.071
51. CR (9)Sb 47	1055. RY (1)Sb 47	0.92	2.67	0.044
51. CR (9)Sb 47	1056. RY (2)Sb 47	6.88	2.59	0.119
51. CR (9)Sb 47	1057. RY (3)Sb 47	4.00	2.50	0.089
51. CR (9)Sb 47	1060. RY (6)Sb 47	2.16	2.58	0.067
51. CR (9)Sb 47	1061. RY (7)Sb 47	2.04	3.02	0.070
51. CR (9)Sb 47	1062. RY (8)Sb 47	0.60	2.46	0.034
51. CR (9)Sb 47	1078. RY (24)Sb 47	1.80	4.08	0.076
51. CR (9)Sb 47	1082. RY (28)Sb 47	0.55	3.98	0.042
51. CR (9)Sb 47	1084. RY (30)Sb 47	1.94	6.79	0.102
51. CR (9)Sb 47	1085. RY (31)Sb 47	2.06	3.47	0.075
67. CR (1)C1 51	1203. RY (28)C1 51	1.21	120.91	0.342
68. CR (2)C1 51	1185. RY (10)C1 51	1.52	17.71	0.146
68. CR (2)C1 51	1198. RY (23)C1 51	0.67	24.46	0.114
68. CR (2)C1 51	1203. RY (28)C1 51	6.06	32.83	0.398
69. CR (3)C1 51	240. BD* (1)Sb 47-C1 51	1.92	8.56	0.114
69. CR (3)C1 51	1176. RY (1)C1 51	0.70	9.79	0.074
69. CR (3)C1 51	1181. RY (6)C1 51	0.90	9.94	0.084
69. CR (3)C1 51	1184. RY (9)C1 51	0.56	9.56	0.065
69. CR (3)C1 51	1185. RY (10)C1 51	1.48	11.69	0.117
69. CR (3)C1 51	1193. RY (18)C1 51	1.72	11.31	0.124
69. CR (3)C1 51	1194. RY (19)C1 51	1.44	10.22	0.108
69. CR (3)C1 51	1196. RY (21)C1 51	1.33	17.02	0.134
69. CR (3)C1 51	1197. RY (22)C1 51	10.23	16.32	0.365
69. CR (3)C1 51	1198. RY (23)C1 51	8.34	18.44	0.350
69. CR (3)C1 51	1199. RY (24)C1 51	0.88	11.22	0.089
70. CR (4)C1 51	240. BD* (1)Sb 47-C1 51	1.18	8.55	0.090
70. CR (4)C1 51	1178. RY (3)C1 51	0.73	9.12	0.073
70. CR (4)C1 51	1181. RY (6)C1 51	0.82	9.94	0.080
70. CR (4)C1 51	1185. RY (10)C1 51	1.61	11.69	0.122
70. CR (4)C1 51	1193. RY (18)C1 51	1.16	11.31	0.102
70. CR (4)C1 51	1194. RY (19)C1 51	0.77	10.22	0.079
70. CR (4)C1 51	1196. RY (21)C1 51	12.05	17.02	0.404
70. CR (4)C1 51	1197. RY (22)C1 51	10.32	16.31	0.366
70. CR (4)C1 51	1198. RY (23)C1 51	0.69	18.44	0.101
71. CR (5)C1 51	1179. RY (4)C1 51	0.76	9.14	0.075
71. CR (5)C1 51	1182. RY (7)C1 51	1.30	9.56	0.099
71. CR (5)C1 51	1191. RY (16)C1 51	0.82	10.23	0.082
71. CR (5)C1 51	1192. RY (17)C1 51	1.63	10.25	0.115
71. CR (5)C1 51	1196. RY (21)C1 51	9.72	17.02	0.363
71. CR (5)C1 51	1197. RY (22)C1 51	5.43	16.31	0.266
71. CR (5)C1 51	1198. RY (23)C1 51	8.50	18.44	0.353
96. LP (1)Sb 47	240. BD* (1)Sb 47-C1 51	8.03	0.48	0.056
96. LP (1)Sb 47	1055. RY (1)Sb 47	0.66	1.27	0.026
96. LP (1)Sb 47	1070. RY (16)Sb 47	0.74	5.02	0.055

96. LP (1)Sb 47	1071. RY (17)Sb 47	0.75	2.12	0.035
96. LP (1)Sb 47	1072. RY (18)Sb 47	1.80	2.23	0.057
96. LP (1)Sb 47	1073. RY (19)Sb 47	1.46	2.49	0.054
96. LP (1)Sb 47	1076. RY (22)Sb 47	0.68	10.16	0.074
109. LP (1)Cl 51	240. BD*(1)Sb 47-cl 51	0.52	0.81	0.018
109. LP (1)Cl 51	1055. RY (1)Sb 47	0.53	1.59	0.026
109. LP (1)Cl 51	1176. RY (1)Cl 51	4.52	2.05	0.086
109. LP (1)Cl 51	1181. RY (6)Cl 51	5.64	2.19	0.099
109. LP (1)Cl 51	1182. RY (7)Cl 51	1.54	1.81	0.047
109. LP (1)Cl 51	1185. RY (10)Cl 51	0.69	3.95	0.047
109. LP (1)Cl 51	1198. RY (23)Cl 51	1.07	10.70	0.096
109. LP (1)Cl 51	1203. RY (28)Cl 51	1.45	19.07	0.149
110. LP (2)Cl 51	182. LV (1)Sb 47	1.04	0.32	0.016
110. LP (2)Cl 51	183. LV (2)Sb 47	3.29	0.32	0.029
110. LP (2)Cl 51	1071. RY (17)Sb 47	0.66	2.00	0.032
110. LP (2)Cl 51	1178. RY (3)Cl 51	9.27	0.92	0.083
110. LP (2)Cl 51	1182. RY (7)Cl 51	0.82	1.37	0.030
110. LP (2)Cl 51	1183. RY (8)Cl 51	0.82	0.95	0.025
110. LP (2)Cl 51	1184. RY (9)Cl 51	7.45	1.36	0.090
110. LP (2)Cl 51	1192. RY (17)Cl 51	0.87	2.05	0.038
110. LP (2)Cl 51	1194. RY (19)Cl 51	4.63	2.02	0.086
110. LP (2)Cl 51	1196. RY (21)Cl 51	2.06	8.83	0.120
110. LP (2)Cl 51	1197. RY (22)Cl 51	2.82	8.12	0.135
110. LP (2)Cl 51	1198. RY (23)Cl 51	0.50	10.25	0.064
111. LP (3)Cl 51	182. LV (1)Sb 47	3.38	0.32	0.029
111. LP (3)Cl 51	183. LV (2)Sb 47	1.08	0.32	0.017
111. LP (3)Cl 51	1058. RY (4)Sb 47	0.59	0.90	0.021
111. LP (3)Cl 51	1179. RY (4)Cl 51	6.86	0.95	0.072
111. LP (3)Cl 51	1181. RY (6)Cl 51	1.31	1.75	0.043
111. LP (3)Cl 51	1182. RY (7)Cl 51	7.95	1.36	0.093
111. LP (3)Cl 51	1184. RY (9)Cl 51	1.83	1.36	0.045
111. LP (3)Cl 51	1191. RY (16)Cl 51	2.80	2.04	0.067
111. LP (3)Cl 51	1192. RY (17)Cl 51	2.49	2.05	0.064
111. LP (3)Cl 51	1196. RY (21)Cl 51	2.00	8.83	0.119
111. LP (3)Cl 51	1197. RY (22)Cl 51	2.92	8.12	0.137
111. LP (3)Cl 51	1198. RY (23)Cl 51	0.50	10.25	0.064
173. BD (1)Sb 47-cl 51	240. BD*(1)Sb 47-cl 51	13.03	0.54	0.075
173. BD (1)Sb 47-cl 51	1055. RY (1)Sb 47	0.64	1.32	0.026
173. BD (1)Sb 47-cl 51	1059. RY (5)Sb 47	0.65	1.71	0.030
173. BD (1)Sb 47-cl 51	1176. RY (1)Cl 51	1.81	1.78	0.051
173. BD (1)Sb 47-cl 51	1177. RY (2)Cl 51	1.74	2.63	0.060
173. BD (1)Sb 47-cl 51	1181. RY (6)Cl 51	1.60	1.92	0.049
173. BD (1)Sb 47-cl 51	1182. RY (7)Cl 51	0.59	1.54	0.027
173. BD (1)Sb 47-cl 51	1185. RY (10)Cl 51	1.95	3.68	0.076
173. BD (1)Sb 47-cl 51	1198. RY (23)Cl 51	0.88	10.43	0.085
from unit 3 to unit 4				
96. LP (1)Sb 47	1092. RY (1)Cl 48	0.66	1.16	0.025
96. LP (1)Sb 47	1093. RY (2)Cl 48	0.16	1.58	0.014
96. LP (1)Sb 47	1095. RY (4)Cl 48	0.13	1.30	0.011
96. LP (1)Sb 47	1096. RY (5)Cl 48	0.08	1.68	0.010
96. LP (1)Sb 47	1099. RY (8)Cl 48	0.24	3.16	0.025
96. LP (1)Sb 47	1100. RY (9)Cl 48	0.11	1.37	0.011
96. LP (1)Sb 47	1115. RY (24)Cl 48	0.06	15.40	0.028
111. LP (3)Cl 51	1092. RY (1)Cl 48	0.07	1.03	0.007
173. BD (1)Sb 47-cl 51	1093. RY (2)Cl 48	0.28	1.64	0.019
173. BD (1)Sb 47-cl 51	1096. RY (5)Cl 48	0.13	1.74	0.013
from unit 3 to unit 5				
43. CR (1)Sb 47	1124. RY (5)Cl 49	0.06	8.23	0.019
96. LP (1)Sb 47	1120. RY (1)Cl 49	0.63	1.14	0.024
96. LP (1)Sb 47	1121. RY (2)Cl 49	0.12	1.46	0.012
96. LP (1)Sb 47	1122. RY (3)Cl 49	0.05	1.16	0.007
96. LP (1)Sb 47	1124. RY (5)Cl 49	0.17	2.19	0.017
96. LP (1)Sb 47	1125. RY (6)Cl 49	0.09	1.39	0.010
96. LP (1)Sb 47	1126. RY (7)Cl 49	0.06	1.64	0.009
96. LP (1)Sb 47	1127. RY (8)Cl 49	0.31	2.85	0.027
96. LP (1)Sb 47	1128. RY (9)Cl 49	0.11	1.46	0.011
96. LP (1)Sb 47	1130. RY (11)Cl 49	0.07	4.08	0.015
96. LP (1)Sb 47	1138. RY (19)Cl 49	0.07	2.82	0.012
96. LP (1)Sb 47	1144. RY (25)Cl 49	0.06	12.61	0.024
110. LP (2)Cl 51	1120. RY (1)Cl 49	0.08	1.02	0.008
110. LP (2)Cl 51	1121. RY (2)Cl 49	0.05	1.34	0.007
173. BD (1)Sb 47-cl 51	1121. RY (2)Cl 49	0.39	1.52	0.022
173. BD (1)Sb 47-cl 51	1123. RY (4)Cl 49	0.06	1.22	0.008
173. BD (1)Sb 47-cl 51	1124. RY (5)Cl 49	0.21	2.25	0.020
173. BD (1)Sb 47-cl 51	1135. RY (16)Cl 49	0.06	3.31	0.012
from unit 3 to unit 6				
96. LP (1)Sb 47	1148. RY (1)Cl 50	0.52	1.18	0.022
96. LP (1)Sb 47	1149. RY (2)Cl 50	0.08	1.47	0.010
96. LP (1)Sb 47	1152. RY (5)Cl 50	0.07	1.69	0.010
96. LP (1)Sb 47	1153. RY (6)Cl 50	0.09	1.58	0.011
96. LP (1)Sb 47	1154. RY (7)Cl 50	0.14	1.67	0.014
96. LP (1)Sb 47	1155. RY (8)Cl 50	0.21	2.59	0.021
96. LP (1)Sb 47	1156. RY (9)Cl 50	0.18	1.74	0.016
96. LP (1)Sb 47	1157. RY (10)Cl 50	0.06	4.16	0.014
96. LP (1)Sb 47	1173. RY (26)Cl 50	0.05	7.33	0.018
111. LP (3)Cl 51	1148. RY (1)Cl 50	0.08	1.05	0.008
173. BD (1)Sb 47-cl 51	1149. RY (2)Cl 50	0.25	1.53	0.017
173. BD (1)Sb 47-cl 51	1151. RY (4)Cl 50	0.15	1.23	0.012
173. BD (1)Sb 47-cl 51	1152. RY (5)Cl 50	0.07	1.74	0.010
from unit 3 to unit 7				
96. LP (1)Sb 47	1204. RY (1)Cl 52	0.70	1.20	0.026
96. LP (1)Sb 47	1205. RY (2)Cl 52	0.23	1.88	0.019
96. LP (1)Sb 47	1208. RY (5)Cl 52	0.26	2.63	0.023
96. LP (1)Sb 47	1211. RY (8)Cl 52	0.12	1.75	0.013
96. LP (1)Sb 47	1212. RY (9)Cl 52	0.11	1.69	0.012
96. LP (1)Sb 47	1214. RY (11)Cl 52	0.07	4.36	0.016
96. LP (1)Sb 47	1227. RY (24)Cl 52	0.06	14.05	0.026
110. LP (2)Cl 51	1204. RY (1)Cl 52	0.07	1.08	0.008
110. LP (2)Cl 51	1210. RY (7)Cl 52	0.08	2.20	0.012

173. BD (1)Sb 47-C1 51	1205. RY (2)C1 52	0.22	1.94	0.018
173. BD (1)Sb 47-C1 51	1208. RY (5)C1 52	0.11	2.68	0.015
from unit 3 to unit 8				
None above threshold				
from unit 4 to unit 1				
99. LP (3)C1 48	251. RY (4)Pt 1	0.05	2.18	0.010
99. LP (3)C1 48	256. RY (9)Pt 1	0.08	2.65	0.013
from unit 4 to unit 2				
98. LP (2)C1 48	588. RY (4) C 16	0.08	1.62	0.010
98. LP (2)C1 48	611. RY (1) C 17	0.11	2.45	0.015
98. LP (2)C1 48	613. RY (3) C 17	0.10	1.39	0.010
98. LP (2)C1 48	620. RY (10) C 17	0.06	2.98	0.012
98. LP (2)C1 48	622. RY (12) C 17	0.06	3.41	0.012
99. LP (3)C1 48	196. BD* (2) N 7- C 10	0.50	0.14	0.007
99. LP (3)C1 48	492. RY (1) C 10	0.06	1.86	0.009
99. LP (3)C1 48	493. RY (2) C 10	0.32	1.32	0.018
99. LP (3)C1 48	496. RY (5) C 10	0.05	2.32	0.010
99. LP (3)C1 48	498. RY (7) C 10	0.30	1.71	0.020
99. LP (3)C1 48	501. RY (10) C 10	0.06	2.33	0.010
99. LP (3)C1 48	504. RY (13) C 10	0.25	2.84	0.024
99. LP (3)C1 48	525. RY (3) C 12	0.06	1.07	0.007
from unit 4 to unit 3				
53. CR (2)C1 48	182. LV (1)Sb 47	0.25	14.85	0.054
53. CR (2)C1 48	1058. RY (4)Sb 47	0.31	15.43	0.062
53. CR (2)C1 48	1063. RY (9)Sb 47	0.06	16.03	0.027
54. CR (3)C1 48	1057. RY (3)Sb 47	0.09	9.14	0.026
54. CR (3)C1 48	1060. RY (6)Sb 47	0.05	9.22	0.019
55. CR (4)C1 48	1057. RY (3)Sb 47	0.06	9.14	0.020
55. CR (4)C1 48	1062. RY (8)Sb 47	0.05	9.10	0.020
56. CR (5)C1 48	182. LV (1)Sb 47	0.12	8.49	0.029
56. CR (5)C1 48	1055. RY (1)Sb 47	0.07	9.32	0.023
56. CR (5)C1 48	1056. RY (2)Sb 47	0.24	9.23	0.042
56. CR (5)C1 48	1057. RY (3)Sb 47	0.07	9.14	0.022
56. CR (5)C1 48	1063. RY (9)Sb 47	0.30	9.66	0.048
56. CR (5)C1 48	1068. RY (14)Sb 47	0.13	9.63	0.031
56. CR (5)C1 48	1070. RY (16)Sb 47	0.12	13.07	0.035
56. CR (5)C1 48	1074. RY (20)Sb 47	0.11	10.34	0.030
56. CR (5)C1 48	1084. RY (30)Sb 47	0.17	13.44	0.042
97. LP (1)C1 48	182. LV (1)Sb 47	6.97	0.73	0.064
97. LP (1)C1 48	183. LV (2)Sb 47	1.24	0.73	0.027
97. LP (1)C1 48	240. BD* (1)Sb 47-C1 51	0.06	0.78	0.006
97. LP (1)C1 48	1056. RY (2)Sb 47	0.09	1.47	0.010
97. LP (1)C1 48	1058. RY (4)Sb 47	0.20	1.31	0.015
97. LP (1)C1 48	1067. RY (13)Sb 47	0.10	1.97	0.012
97. LP (1)C1 48	1068. RY (14)Sb 47	0.15	1.88	0.015
97. LP (1)C1 48	1072. RY (18)Sb 47	0.32	2.52	0.026
97. LP (1)C1 48	1073. RY (19)Sb 47	0.51	2.79	0.034
97. LP (1)C1 48	1076. RY (22)Sb 47	0.07	10.45	0.024
97. LP (1)C1 48	1077. RY (23)Sb 47	0.15	2.37	0.017
97. LP (1)C1 48	1090. RY (36)Sb 47	0.08	37.07	0.047
98. LP (2)C1 48	182. LV (1)Sb 47	1.32	0.30	0.018
98. LP (2)C1 48	183. LV (2)Sb 47	0.79	0.30	0.014
98. LP (2)C1 48	240. BD* (1)Sb 47-C1 51	0.12	0.35	0.006
98. LP (2)C1 48	1057. RY (3)Sb 47	0.18	0.96	0.012
98. LP (2)C1 48	1058. RY (4)Sb 47	0.16	0.89	0.011
98. LP (2)C1 48	1064. RY (10)Sb 47	0.09	2.25	0.013
98. LP (2)C1 48	1069. RY (15)Sb 47	0.13	1.40	0.012
98. LP (2)C1 48	1071. RY (17)Sb 47	0.30	1.98	0.022
98. LP (2)C1 48	1082. RY (28)Sb 47	0.06	2.44	0.010
98. LP (2)C1 48	1085. RY (31)Sb 47	0.20	1.93	0.017
98. LP (2)C1 48	1091. RY (37)Sb 47	0.08	36.77	0.048
99. LP (3)C1 48	183. LV (2)Sb 47	0.37	0.30	0.009
99. LP (3)C1 48	240. BD* (1)Sb 47-C1 51	1.02	0.35	0.017
99. LP (3)C1 48	1057. RY (3)Sb 47	0.05	0.95	0.006
99. LP (3)C1 48	1058. RY (4)Sb 47	0.31	0.88	0.015
99. LP (3)C1 48	1059. RY (5)Sb 47	0.11	1.52	0.012
99. LP (3)C1 48	1067. RY (13)Sb 47	0.21	1.54	0.016
99. LP (3)C1 48	1072. RY (18)Sb 47	0.08	2.09	0.012
99. LP (3)C1 48	1073. RY (19)Sb 47	0.10	2.36	0.013
99. LP (3)C1 48	1074. RY (20)Sb 47	0.18	2.16	0.018
99. LP (3)C1 48	1075. RY (21)Sb 47	0.11	2.84	0.015
99. LP (3)C1 48	1086. RY (32)Sb 47	0.05	33.27	0.037
99. LP (3)C1 48	1179. RY (4)C1 51	0.06	0.94	0.007
99. LP (3)C1 48	1181. RY (6)C1 51	0.12	1.73	0.013
100. LP (4)C1 48	182. LV (1)Sb 47	41.14	0.40	0.115
100. LP (4)C1 48	183. LV (2)Sb 47	7.03	0.40	0.048
100. LP (4)C1 48	240. BD* (1)Sb 47-C1 51	1.53	0.45	0.023
100. LP (4)C1 48	1055. RY (1)Sb 47	0.06	1.23	0.008
100. LP (4)C1 48	1057. RY (3)Sb 47	0.14	1.06	0.011
100. LP (4)C1 48	1059. RY (5)Sb 47	1.03	1.62	0.037
100. LP (4)C1 48	1060. RY (6)Sb 47	0.31	1.14	0.017
100. LP (4)C1 48	1061. RY (7)Sb 47	0.92	1.58	0.034
100. LP (4)C1 48	1062. RY (8)Sb 47	0.24	1.02	0.014
100. LP (4)C1 48	1064. RY (10)Sb 47	0.95	2.35	0.042
100. LP (4)C1 48	1065. RY (11)Sb 47	0.76	2.60	0.040
100. LP (4)C1 48	1066. RY (12)Sb 47	0.45	1.67	0.024
100. LP (4)C1 48	1067. RY (13)Sb 47	0.52	1.65	0.026
100. LP (4)C1 48	1070. RY (16)Sb 47	1.15	4.99	0.067
100. LP (4)C1 48	1071. RY (17)Sb 47	0.06	2.08	0.010
100. LP (4)C1 48	1072. RY (18)Sb 47	0.13	2.19	0.015
100. LP (4)C1 48	1074. RY (20)Sb 47	0.68	2.26	0.035
100. LP (4)C1 48	1075. RY (21)Sb 47	0.22	2.94	0.022
100. LP (4)C1 48	1076. RY (22)Sb 47	0.30	10.13	0.049
100. LP (4)C1 48	1078. RY (24)Sb 47	0.28	2.64	0.024
100. LP (4)C1 48	1079. RY (25)Sb 47	0.25	2.89	0.024
100. LP (4)C1 48	1080. RY (26)Sb 47	0.39	4.33	0.037
100. LP (4)C1 48	1081. RY (27)Sb 47	0.35	8.03	0.047
100. LP (4)C1 48	1083. RY (29)Sb 47	0.91	33.84	0.157
100. LP (4)C1 48	1084. RY (30)Sb 47	1.99	5.36	0.092

100. LP (4)C1 48	1087. RY (33)Sb 47	0.44	8.16	0.053
100. LP (4)C1 48	1088. RY (34)Sb 47	0.15	5.84	0.026
100. LP (4)C1 48	1089. RY (35)Sb 47	0.25	93.67	0.135
100. LP (4)C1 48	1090. RY (36)Sb 47	0.93	36.75	0.165
100. LP (4)C1 48	1091. RY (37)Sb 47	0.27	36.87	0.088
100. LP (4)C1 48	1177. RY (2)C1 51	0.06	2.54	0.011
within unit 4				
52. CR (1)C1 48	1115. RY (24)C1 48	1.09	117.20	0.318
53. CR (2)C1 48	1101. RY (10)C1 48	0.98	17.59	0.117
53. CR (2)C1 48	1102. RY (11)C1 48	1.66	18.64	0.157
53. CR (2)C1 48	1115. RY (24)C1 48	5.55	29.82	0.363
53. CR (2)C1 48	1117. RY (26)C1 48	0.70	18.25	0.101
54. CR (3)C1 48	1096. RY (5)C1 48	1.07	9.73	0.091
54. CR (3)C1 48	1105. RY (14)C1 48	0.71	11.34	0.080
54. CR (3)C1 48	1106. RY (15)C1 48	0.70	10.56	0.077
54. CR (3)C1 48	1107. RY (16)C1 48	0.62	11.22	0.074
54. CR (3)C1 48	1108. RY (17)C1 48	0.84	11.44	0.087
54. CR (3)C1 48	1109. RY (18)C1 48	0.82	11.52	0.087
54. CR (3)C1 48	1110. RY (19)C1 48	8.59	17.42	0.345
54. CR (3)C1 48	1111. RY (20)C1 48	6.67	17.25	0.303
54. CR (3)C1 48	1112. RY (21)C1 48	5.79	17.59	0.285
54. CR (3)C1 48	1113. RY (22)C1 48	1.11	10.92	0.098
54. CR (3)C1 48	1114. RY (23)C1 48	1.74	11.39	0.126
55. CR (4)C1 48	1097. RY (6)C1 48	0.95	9.43	0.085
55. CR (4)C1 48	1105. RY (14)C1 48	1.80	11.34	0.127
55. CR (4)C1 48	1106. RY (15)C1 48	0.61	10.56	0.072
55. CR (4)C1 48	1109. RY (18)C1 48	0.88	11.52	0.090
55. CR (4)C1 48	1110. RY (19)C1 48	5.91	17.42	0.286
55. CR (4)C1 48	1111. RY (20)C1 48	15.58	17.25	0.463
55. CR (4)C1 48	1112. RY (21)C1 48	1.47	17.59	0.143
55. CR (4)C1 48	1116. RY (25)C1 48	0.59	10.94	0.072
56. CR (5)C1 48	1092. RY (1)C1 48	0.81	9.20	0.077
56. CR (5)C1 48	1098. RY (7)C1 48	1.50	10.02	0.109
56. CR (5)C1 48	1099. RY (8)C1 48	0.66	11.21	0.077
56. CR (5)C1 48	1101. RY (10)C1 48	2.27	11.22	0.142
56. CR (5)C1 48	1102. RY (11)C1 48	0.86	12.28	0.092
56. CR (5)C1 48	1110. RY (19)C1 48	8.13	17.42	0.336
56. CR (5)C1 48	1112. RY (21)C1 48	11.93	17.60	0.409
56. CR (5)C1 48	1114. RY (23)C1 48	0.62	11.40	0.075
97. LP (1)C1 48	1096. RY (5)C1 48	0.59	1.97	0.031
97. LP (1)C1 48	1098. RY (7)C1 48	6.47	2.27	0.108
97. LP (1)C1 48	1099. RY (8)C1 48	1.11	3.45	0.055
97. LP (1)C1 48	1101. RY (10)C1 48	1.12	3.47	0.056
97. LP (1)C1 48	1102. RY (11)C1 48	0.79	4.52	0.053
97. LP (1)C1 48	1107. RY (16)C1 48	0.89	3.47	0.050
97. LP (1)C1 48	1112. RY (21)C1 48	0.80	9.84	0.079
97. LP (1)C1 48	1115. RY (24)C1 48	1.98	15.70	0.157
98. LP (2)C1 48	1094. RY (3)C1 48	1.76	0.94	0.036
98. LP (2)C1 48	1095. RY (4)C1 48	2.47	1.16	0.048
98. LP (2)C1 48	1096. RY (5)C1 48	1.67	1.55	0.045
98. LP (2)C1 48	1097. RY (6)C1 48	10.34	1.25	0.102
98. LP (2)C1 48	1100. RY (9)C1 48	1.25	1.23	0.035
98. LP (2)C1 48	1105. RY (14)C1 48	2.66	3.16	0.082
98. LP (2)C1 48	1106. RY (15)C1 48	1.31	2.38	0.050
98. LP (2)C1 48	1110. RY (19)C1 48	0.66	9.24	0.070
98. LP (2)C1 48	1111. RY (20)C1 48	3.55	9.07	0.160
98. LP (2)C1 48	1113. RY (22)C1 48	0.84	2.73	0.043
99. LP (3)C1 48	1093. RY (2)C1 48	1.66	1.44	0.044
99. LP (3)C1 48	1094. RY (3)C1 48	0.54	0.94	0.020
99. LP (3)C1 48	1095. RY (4)C1 48	1.62	1.16	0.039
99. LP (3)C1 48	1096. RY (5)C1 48	7.15	1.55	0.094
99. LP (3)C1 48	1097. RY (6)C1 48	2.55	1.25	0.050
99. LP (3)C1 48	1098. RY (7)C1 48	1.22	1.84	0.042
99. LP (3)C1 48	1100. RY (9)C1 48	0.69	1.23	0.026
99. LP (3)C1 48	1108. RY (17)C1 48	0.54	3.25	0.037
99. LP (3)C1 48	1109. RY (18)C1 48	1.17	3.34	0.056
99. LP (3)C1 48	1110. RY (19)C1 48	3.48	9.23	0.160
99. LP (3)C1 48	1111. RY (20)C1 48	0.85	9.07	0.079
99. LP (3)C1 48	1117. RY (26)C1 48	0.61	3.70	0.042
100. LP (4)C1 48	1092. RY (1)C1 48	5.05	1.12	0.067
100. LP (4)C1 48	1093. RY (2)C1 48	1.46	1.55	0.042
100. LP (4)C1 48	1096. RY (5)C1 48	1.24	1.65	0.040
100. LP (4)C1 48	1098. RY (7)C1 48	0.94	1.94	0.038
100. LP (4)C1 48	1101. RY (10)C1 48	2.94	3.14	0.086
100. LP (4)C1 48	1102. RY (11)C1 48	1.46	4.20	0.070
100. LP (4)C1 48	1112. RY (21)C1 48	3.00	9.52	0.151
100. LP (4)C1 48	1114. RY (23)C1 48	0.57	3.32	0.039
from unit 4 to unit 5				
98. LP (2)C1 48	1127. RY (8)C1 49	0.07	2.71	0.012
from unit 4 to unit 6				
100. LP (4)C1 48	1152. RY (5)C1 50	0.15	1.65	0.014
100. LP (4)C1 48	1157. RY (10)C1 50	0.21	4.12	0.026
from unit 4 to unit 7				
None above threshold				
from unit 4 to unit 8				
None above threshold				
from unit 5 to unit 1				
60. CR (4)C1 49	284. RY (7) S 2	0.05	10.04	0.020
102. LP (2)C1 49	228. BD*(1) C 32- H 33	0.22	0.77	0.012
102. LP (2)C1 49	875. RY (1) C 32	0.05	1.48	0.008
102. LP (2)C1 49	901. RY (1) H 33	0.43	1.67	0.024
102. LP (2)C1 49	902. RY (2) H 33	0.15	2.27	0.016
103. LP (3)C1 49	187. BD*(1) S 2- C 44	0.57	0.32	0.012
103. LP (3)C1 49	225. BD*(1) C 29- H 30	0.08	0.74	0.007
103. LP (3)C1 49	228. BD*(1) C 32- H 33	0.15	0.80	0.010
103. LP (3)C1 49	251. RY (4)Pt 1	0.07	2.22	0.011
103. LP (3)C1 49	254. RY (7)Pt 1	0.12	2.00	0.014

103. LP (3)C1 49	255. RY (8)Pt 1	0.06	2.61	0.012
103. LP (3)C1 49	260. RY (13)Pt 1	0.06	7.37	0.018
103. LP (3)C1 49	282. RY (5) S 2	0.06	5.11	0.015
103. LP (3)C1 49	284. RY (7) S 2	0.41	1.89	0.025
103. LP (3)C1 49	285. RY (8) S 2	0.06	1.99	0.010
103. LP (3)C1 49	293. RY (16) S 2	0.08	3.07	0.014
103. LP (3)C1 49	839. RY (1) C 29	0.06	1.56	0.009
103. LP (3)C1 49	842. RY (4) C 29	0.11	1.88	0.013
103. LP (3)C1 49	901. RY (1) H 33	0.28	1.70	0.020
103. LP (3)C1 49	902. RY (2) H 33	0.14	2.30	0.016
104. LP (4)C1 49	248. RY (1)Pt 1	0.05	2.24	0.010

from unit 5 to unit 2
None above threshold

from unit 5 to unit 3

58. CR (2)C1 49	183. LV (2)Sb 47	0.22	14.90	0.051
58. CR (2)C1 49	1057. RY (3)Sb 47	0.32	15.55	0.063
58. CR (2)C1 49	1065. RY (11)Sb 47	0.05	17.10	0.027
58. CR (2)C1 49	1070. RY (16)Sb 47	0.06	19.48	0.029
58. CR (2)C1 49	1084. RY (30)Sb 47	0.05	19.85	0.028
59. CR (3)C1 49	183. LV (2)Sb 47	0.06	8.50	0.020
59. CR (3)C1 49	1056. RY (2)Sb 47	0.11	9.24	0.028
59. CR (3)C1 49	1065. RY (11)Sb 47	0.11	10.70	0.031
59. CR (3)C1 49	1066. RY (12)Sb 47	0.06	9.76	0.022
59. CR (3)C1 49	1070. RY (16)Sb 47	0.05	13.08	0.023
59. CR (3)C1 49	1071. RY (17)Sb 47	0.06	10.18	0.022
59. CR (3)C1 49	1084. RY (30)Sb 47	0.08	13.45	0.029
60. CR (4)C1 49	183. LV (2)Sb 47	0.08	8.50	0.024
60. CR (4)C1 49	1055. RY (1)Sb 47	0.12	9.33	0.030
60. CR (4)C1 49	1056. RY (2)Sb 47	0.16	9.24	0.035
60. CR (4)C1 49	1057. RY (3)Sb 47	0.07	9.15	0.023
60. CR (4)C1 49	1065. RY (11)Sb 47	0.17	10.70	0.039
60. CR (4)C1 49	1066. RY (12)Sb 47	0.06	9.76	0.021
60. CR (4)C1 49	1067. RY (13)Sb 47	0.07	9.74	0.024
60. CR (4)C1 49	1069. RY (15)Sb 47	0.05	9.60	0.020
60. CR (4)C1 49	1070. RY (16)Sb 47	0.06	13.09	0.026
60. CR (4)C1 49	1078. RY (24)Sb 47	0.06	10.74	0.023
60. CR (4)C1 49	1084. RY (30)Sb 47	0.17	13.45	0.042
61. CR (5)C1 49	1058. RY (4)Sb 47	0.09	9.08	0.026
61. CR (5)C1 49	1062. RY (8)Sb 47	0.08	9.11	0.024
101. LP (1)C1 49	182. LV (1)Sb 47	1.28	0.73	0.027
101. LP (1)C1 49	183. LV (2)Sb 47	7.17	0.73	0.064
101. LP (1)C1 49	240. BD* (1)Sb 47-cl 51	0.19	0.77	0.011
101. LP (1)C1 49	1056. RY (2)Sb 47	0.21	1.47	0.016
101. LP (1)C1 49	1057. RY (3)Sb 47	0.09	1.38	0.010
101. LP (1)C1 49	1065. RY (11)Sb 47	0.07	2.92	0.013
101. LP (1)C1 49	1069. RY (15)Sb 47	0.23	1.82	0.018
101. LP (1)C1 49	1071. RY (17)Sb 47	0.51	2.41	0.031
101. LP (1)C1 49	1072. RY (18)Sb 47	0.36	2.52	0.027
101. LP (1)C1 49	1074. RY (20)Sb 47	0.06	2.58	0.011
101. LP (1)C1 49	1076. RY (22)Sb 47	0.07	10.45	0.024
101. LP (1)C1 49	1080. RY (26)Sb 47	0.05	4.65	0.014
101. LP (1)C1 49	1081. RY (27)Sb 47	0.06	8.35	0.020
101. LP (1)C1 49	1083. RY (29)Sb 47	0.07	34.17	0.043
101. LP (1)C1 49	1084. RY (30)Sb 47	0.06	5.68	0.016
101. LP (1)C1 49	1091. RY (37)Sb 47	0.06	37.20	0.041
102. LP (2)C1 49	182. LV (1)Sb 47	2.02	0.31	0.022
102. LP (2)C1 49	183. LV (2)Sb 47	0.16	0.31	0.006
102. LP (2)C1 49	1058. RY (4)Sb 47	0.32	0.90	0.015
102. LP (2)C1 49	1063. RY (9)Sb 47	0.18	1.49	0.015
102. LP (2)C1 49	1068. RY (14)Sb 47	0.14	1.46	0.013
102. LP (2)C1 49	1072. RY (18)Sb 47	0.14	2.10	0.015
102. LP (2)C1 49	1073. RY (19)Sb 47	0.14	2.37	0.016
102. LP (2)C1 49	1085. RY (31)Sb 47	0.28	1.94	0.021
102. LP (2)C1 49	1090. RY (36)Sb 47	0.07	36.66	0.044
103. LP (3)C1 49	182. LV (1)Sb 47	0.44	0.34	0.011
103. LP (3)C1 49	183. LV (2)Sb 47	1.18	0.34	0.018
103. LP (3)C1 49	240. BD* (1)Sb 47-cl 51	0.95	0.39	0.017
103. LP (3)C1 49	1056. RY (2)Sb 47	0.20	1.09	0.013
103. LP (3)C1 49	1057. RY (3)Sb 47	0.48	1.00	0.019
103. LP (3)C1 49	1061. RY (7)Sb 47	0.09	1.52	0.010
103. LP (3)C1 49	1066. RY (12)Sb 47	0.24	1.60	0.018
103. LP (3)C1 49	1071. RY (17)Sb 47	0.23	2.02	0.019
103. LP (3)C1 49	1073. RY (19)Sb 47	0.06	2.40	0.011
103. LP (3)C1 49	1086. RY (32)Sb 47	0.06	33.31	0.041
103. LP (3)C1 49	1178. RY (3)C1 51	0.10	0.95	0.009
103. LP (3)C1 49	1181. RY (6)C1 51	0.08	1.77	0.011
104. LP (4)C1 49	182. LV (1)Sb 47	9.25	0.43	0.056
104. LP (4)C1 49	183. LV (2)Sb 47	44.73	0.43	0.124
104. LP (4)C1 49	240. BD* (1)Sb 47-cl 51	2.36	0.48	0.030
104. LP (4)C1 49	1055. RY (1)Sb 47	0.16	1.26	0.013
104. LP (4)C1 49	1056. RY (2)Sb 47	0.16	1.18	0.012
104. LP (4)C1 49	1057. RY (3)Sb 47	0.15	1.09	0.012
104. LP (4)C1 49	1059. RY (5)Sb 47	1.33	1.65	0.042
104. LP (4)C1 49	1060. RY (6)Sb 47	0.34	1.17	0.018
104. LP (4)C1 49	1061. RY (7)Sb 47	0.83	1.61	0.033
104. LP (4)C1 49	1062. RY (8)Sb 47	0.26	1.05	0.015
104. LP (4)C1 49	1063. RY (9)Sb 47	0.14	1.61	0.014
104. LP (4)C1 49	1064. RY (10)Sb 47	1.49	2.38	0.053
104. LP (4)C1 49	1065. RY (11)Sb 47	0.36	2.63	0.027
104. LP (4)C1 49	1066. RY (12)Sb 47	0.59	1.69	0.028
104. LP (4)C1 49	1067. RY (13)Sb 47	0.16	1.68	0.015
104. LP (4)C1 49	1068. RY (14)Sb 47	0.07	1.58	0.009
104. LP (4)C1 49	1069. RY (15)Sb 47	0.23	1.53	0.017
104. LP (4)C1 49	1070. RY (16)Sb 47	1.47	5.02	0.077
104. LP (4)C1 49	1071. RY (17)Sb 47	0.17	2.11	0.017
104. LP (4)C1 49	1073. RY (19)Sb 47	0.46	2.49	0.030
104. LP (4)C1 49	1074. RY (20)Sb 47	0.07	2.29	0.012
104. LP (4)C1 49	1075. RY (21)Sb 47	0.34	2.97	0.028
104. LP (4)C1 49	1076. RY (22)Sb 47	0.60	10.16	0.070
104. LP (4)C1 49	1077. RY (23)Sb 47	0.10	2.07	0.013
104. LP (4)C1 49	1078. RY (24)Sb 47	0.19	2.67	0.020

104. LP (4)C1 49	1079. RY (25)Sb 47	0.42	2.92	0.031
104. LP (4)C1 49	1080. RY (26)Sb 47	0.25	4.35	0.030
104. LP (4)C1 49	1081. RY (27)Sb 47	0.82	8.05	0.072
104. LP (4)C1 49	1083. RY (29)Sb 47	1.47	33.87	0.199
104. LP (4)C1 49	1087. RY (33)Sb 47	0.37	8.19	0.049
104. LP (4)C1 49	1088. RY (34)Sb 47	0.52	5.87	0.049
104. LP (4)C1 49	1089. RY (35)Sb 47	0.17	93.70	0.112
104. LP (4)C1 49	1090. RY (36)Sb 47	0.47	36.78	0.118
104. LP (4)C1 49	1091. RY (37)Sb 47	1.30	36.90	0.195
104. LP (4)C1 49	1177. RY (2)C1 51	0.05	2.57	0.011
from unit 5 to unit 4				
None above threshold				
within unit 5				
57. CR (1)C1 49	1144. RY (25)C1 49	0.83	114.39	0.276
58. CR (2)C1 49	1130. RY (11)C1 49	2.11	18.54	0.177
58. CR (2)C1 49	1131. RY (12)C1 49	1.28	19.23	0.140
58. CR (2)C1 49	1134. RY (15)C1 49	0.53	18.26	0.088
58. CR (2)C1 49	1143. RY (24)C1 49	1.04	18.95	0.125
58. CR (2)C1 49	1144. RY (25)C1 49	4.63	27.07	0.316
59. CR (3)C1 49	1120. RY (1)C1 49	0.58	9.20	0.065
59. CR (3)C1 49	1124. RY (5)C1 49	0.53	10.25	0.066
59. CR (3)C1 49	1127. RY (8)C1 49	1.23	10.91	0.103
59. CR (3)C1 49	1130. RY (11)C1 49	0.81	12.14	0.089
59. CR (3)C1 49	1132. RY (13)C1 49	0.53	10.87	0.068
59. CR (3)C1 49	1135. RY (16)C1 49	0.77	11.31	0.083
59. CR (3)C1 49	1136. RY (17)C1 49	1.12	11.26	0.100
59. CR (3)C1 49	1139. RY (20)C1 49	1.37	17.68	0.139
59. CR (3)C1 49	1140. RY (21)C1 49	11.11	17.54	0.394
59. CR (3)C1 49	1141. RY (22)C1 49	9.22	17.72	0.361
60. CR (4)C1 49	1121. RY (2)C1 49	0.62	9.52	0.069
60. CR (4)C1 49	1127. RY (8)C1 49	0.53	10.91	0.068
60. CR (4)C1 49	1130. RY (11)C1 49	1.39	12.14	0.116
60. CR (4)C1 49	1133. RY (14)C1 49	0.68	11.23	0.078
60. CR (4)C1 49	1134. RY (15)C1 49	0.89	11.86	0.092
60. CR (4)C1 49	1135. RY (16)C1 49	0.94	11.31	0.092
60. CR (4)C1 49	1139. RY (20)C1 49	18.25	17.68	0.507
60. CR (4)C1 49	1140. RY (21)C1 49	1.70	17.54	0.154
60. CR (4)C1 49	1142. RY (23)C1 49	0.77	11.11	0.082
60. CR (4)C1 49	1143. RY (24)C1 49	0.55	12.55	0.074
61. CR (5)C1 49	1126. RY (7)C1 49	1.29	9.70	0.100
61. CR (5)C1 49	1133. RY (14)C1 49	2.40	11.23	0.147
61. CR (5)C1 49	1137. RY (18)C1 49	0.65	10.54	0.074
61. CR (5)C1 49	1139. RY (20)C1 49	0.73	17.68	0.102
61. CR (5)C1 49	1140. RY (21)C1 49	9.42	17.54	0.363
61. CR (5)C1 49	1141. RY (22)C1 49	11.66	17.72	0.406
61. CR (5)C1 49	1142. RY (23)C1 49	1.62	11.11	0.120
101. LP (1)C1 49	1125. RY (6)C1 49	2.40	1.67	0.057
101. LP (1)C1 49	1126. RY (7)C1 49	2.91	1.92	0.067
101. LP (1)C1 49	1127. RY (8)C1 49	2.33	3.14	0.076
101. LP (1)C1 49	1128. RY (9)C1 49	2.46	1.74	0.059
101. LP (1)C1 49	1130. RY (11)C1 49	1.17	4.37	0.064
101. LP (1)C1 49	1131. RY (12)C1 49	0.63	5.06	0.051
101. LP (1)C1 49	1135. RY (16)C1 49	0.90	3.54	0.050
101. LP (1)C1 49	1141. RY (22)C1 49	0.91	9.95	0.085
101. LP (1)C1 49	1143. RY (24)C1 49	0.83	4.77	0.056
101. LP (1)C1 49	1144. RY (25)C1 49	1.89	12.89	0.139
102. LP (2)C1 49	1122. RY (3)C1 49	4.29	1.03	0.059
102. LP (2)C1 49	1126. RY (7)C1 49	8.54	1.51	0.101
102. LP (2)C1 49	1127. RY (8)C1 49	1.87	2.73	0.064
102. LP (2)C1 49	1128. RY (9)C1 49	0.81	1.33	0.029
102. LP (2)C1 49	1132. RY (13)C1 49	0.97	2.68	0.045
102. LP (2)C1 49	1133. RY (14)C1 49	2.09	3.04	0.071
102. LP (2)C1 49	1137. RY (18)C1 49	1.08	2.36	0.045
102. LP (2)C1 49	1140. RY (21)C1 49	3.08	9.36	0.152
102. LP (2)C1 49	1141. RY (22)C1 49	1.16	9.54	0.094
102. LP (2)C1 49	1142. RY (23)C1 49	0.72	2.93	0.041
103. LP (3)C1 49	1121. RY (2)C1 49	3.87	1.37	0.065
103. LP (3)C1 49	1123. RY (4)C1 49	4.44	1.07	0.062
103. LP (3)C1 49	1124. RY (5)C1 49	4.59	2.10	0.088
103. LP (3)C1 49	1128. RY (9)C1 49	1.95	1.36	0.046
103. LP (3)C1 49	1133. RY (14)C1 49	1.27	3.07	0.056
103. LP (3)C1 49	1135. RY (16)C1 49	1.45	3.15	0.060
103. LP (3)C1 49	1136. RY (17)C1 49	0.88	3.10	0.047
103. LP (3)C1 49	1139. RY (20)C1 49	2.42	9.52	0.135
103. LP (3)C1 49	1141. RY (22)C1 49	1.21	9.57	0.096
104. LP (4)C1 49	1120. RY (1)C1 49	4.99	1.14	0.067
104. LP (4)C1 49	1121. RY (2)C1 49	1.38	1.46	0.040
104. LP (4)C1 49	1124. RY (5)C1 49	1.28	2.19	0.047
104. LP (4)C1 49	1126. RY (7)C1 49	0.56	1.63	0.027
104. LP (4)C1 49	1128. RY (9)C1 49	0.75	1.45	0.029
104. LP (4)C1 49	1130. RY (11)C1 49	3.06	4.07	0.100
104. LP (4)C1 49	1139. RY (20)C1 49	1.49	9.61	0.107
104. LP (4)C1 49	1140. RY (21)C1 49	0.87	9.47	0.081
104. LP (4)C1 49	1141. RY (22)C1 49	0.98	9.66	0.087
from unit 5 to unit 6				
102. LP (2)C1 49	1148. RY (1)C1 50	0.06	1.05	0.007
from unit 5 to unit 7				
104. LP (4)C1 49	1204. RY (1)C1 52	0.05	1.20	0.007
104. LP (4)C1 49	1208. RY (5)C1 52	0.08	2.62	0.013
104. LP (4)C1 49	1213. RY (10)C1 52	0.20	3.09	0.022
104. LP (4)C1 49	1214. RY (11)C1 52	0.08	4.35	0.017
from unit 5 to unit 8				
None above threshold				
from unit 6 to unit 1				
64. CR (3)C1 50	256. RY (9)Pt 1	0.07	10.84	0.025
65. CR (4)C1 50	256. RY (9)Pt 1	0.05	10.84	0.021
65. CR (4)C1 50	312. RY (7) S 3	0.05	10.21	0.021

105. LP (1)C1 50	255. RY (8)Pt 1	0.05	2.99	0.011
106. LP (2)C1 50	228. BD* (1) C 32- H 33	0.07	0.76	0.007
106. LP (2)C1 50	880. RY (6) C 32	0.06	1.61	0.008
106. LP (2)C1 50	901. RY (1) H 33	0.20	1.66	0.016
106. LP (2)C1 50	902. RY (2) H 33	0.10	2.26	0.013
107. LP (3)C1 50	184. BD* (1)Pt 1- S 2	0.09	0.36	0.005
107. LP (3)C1 50	185. BD* (1)Pt 1- S 3	0.06	0.37	0.004
107. LP (3)C1 50	189. BD* (1) S 3- C 35	0.58	0.30	0.012
107. LP (3)C1 50	228. BD* (1) C 32- H 33	0.05	0.79	0.006
107. LP (3)C1 50	250. RY (3)Pt 1	0.08	2.78	0.013
107. LP (3)C1 50	251. RY (4)Pt 1	0.16	2.21	0.017
107. LP (3)C1 50	254. RY (7)Pt 1	0.07	1.99	0.010
107. LP (3)C1 50	255. RY (8)Pt 1	0.07	2.60	0.012
107. LP (3)C1 50	256. RY (9)Pt 1	0.29	2.69	0.025
107. LP (3)C1 50	258. RY (11)Pt 1	0.10	2.80	0.015
107. LP (3)C1 50	260. RY (13)Pt 1	0.06	7.36	0.019
107. LP (3)C1 50	310. RY (5) S 3	0.06	3.73	0.013
107. LP (3)C1 50	312. RY (7) S 3	0.39	2.05	0.025
107. LP (3)C1 50	313. RY (8) S 3	0.07	1.81	0.010
107. LP (3)C1 50	317. RY (12) S 3	0.11	3.12	0.017
107. LP (3)C1 50	880. RY (6) C 32	0.08	1.64	0.010
107. LP (3)C1 50	901. RY (1) H 33	0.11	1.70	0.012
107. LP (3)C1 50	902. RY (2) H 33	0.06	2.29	0.011
108. LP (4)C1 50	248. RY (1)Pt 1	0.11	2.22	0.014
108. LP (4)C1 50	252. RY (5)Pt 1	0.06	2.76	0.012
108. LP (4)C1 50	253. RY (6)Pt 1	0.07	3.22	0.014
from unit 6 to unit 2				
106. LP (2)C1 50	200. BD* (2) N 8- C 27	0.07	0.16	0.003
106. LP (2)C1 50	809. RY (2) C 27	0.24	1.26	0.016
106. LP (2)C1 50	813. RY (6) C 27	0.10	2.23	0.013
107. LP (3)C1 50	200. BD* (2) N 8- C 27	0.06	0.19	0.003
107. LP (3)C1 50	809. RY (2) C 27	0.11	1.29	0.010
107. LP (3)C1 50	813. RY (6) C 27	0.05	2.26	0.010
from unit 6 to unit 3				
63. CR (2)C1 50	182. LV (1)Sb 47	0.27	14.91	0.056
63. CR (2)C1 50	1056. RY (2)Sb 47	0.10	15.65	0.035
63. CR (2)C1 50	1058. RY (4)Sb 47	0.24	15.49	0.054
64. CR (3)C1 50	1055. RY (1)Sb 47	0.06	9.32	0.021
64. CR (3)C1 50	1056. RY (2)Sb 47	0.10	9.24	0.027
64. CR (3)C1 50	1062. RY (8)Sb 47	0.05	9.11	0.020
65. CR (4)C1 50	1057. RY (3)Sb 47	0.06	9.15	0.020
66. CR (5)C1 50	182. LV (1)Sb 47	0.13	8.49	0.030
66. CR (5)C1 50	1056. RY (2)Sb 47	0.21	9.24	0.040
66. CR (5)C1 50	1057. RY (3)Sb 47	0.11	9.15	0.029
66. CR (5)C1 50	1063. RY (9)Sb 47	0.13	9.67	0.032
66. CR (5)C1 50	1064. RY (10)Sb 47	0.12	10.44	0.031
66. CR (5)C1 50	1067. RY (13)Sb 47	0.11	9.74	0.029
66. CR (5)C1 50	1070. RY (16)Sb 47	0.11	13.08	0.034
66. CR (5)C1 50	1074. RY (20)Sb 47	0.12	10.35	0.031
66. CR (5)C1 50	1078. RY (24)Sb 47	0.06	10.73	0.023
66. CR (5)C1 50	1084. RY (30)Sb 47	0.14	13.44	0.039
105. LP (1)C1 50	182. LV (1)Sb 47	6.63	0.72	0.062
105. LP (1)C1 50	183. LV (2)Sb 47	1.08	0.72	0.025
105. LP (1)C1 50	240. BD* (1)Sb 47-C1 51	0.07	0.77	0.007
105. LP (1)C1 50	1058. RY (4)Sb 47	0.21	1.30	0.015
105. LP (1)C1 50	1063. RY (9)Sb 47	0.05	1.90	0.009
105. LP (1)C1 50	1068. RY (14)Sb 47	0.30	1.87	0.021
105. LP (1)C1 50	1072. RY (18)Sb 47	0.16	2.51	0.018
105. LP (1)C1 50	1073. RY (19)Sb 47	0.29	2.78	0.025
105. LP (1)C1 50	1076. RY (22)Sb 47	0.10	10.44	0.029
105. LP (1)C1 50	1079. RY (25)Sb 47	0.11	3.21	0.017
105. LP (1)C1 50	1083. RY (29)Sb 47	0.05	34.16	0.037
105. LP (1)C1 50	1090. RY (36)Sb 47	0.07	37.06	0.046
106. LP (2)C1 50	182. LV (1)Sb 47	0.28	0.31	0.008
106. LP (2)C1 50	183. LV (2)Sb 47	1.44	0.31	0.019
106. LP (2)C1 50	240. BD* (1)Sb 47-C1 51	0.08	0.35	0.005
106. LP (2)C1 50	1056. RY (2)Sb 47	0.07	1.05	0.008
106. LP (2)C1 50	1057. RY (3)Sb 47	0.18	0.96	0.012
106. LP (2)C1 50	1064. RY (10)Sb 47	0.08	2.25	0.012
106. LP (2)C1 50	1069. RY (15)Sb 47	0.14	1.40	0.012
106. LP (2)C1 50	1071. RY (17)Sb 47	0.30	1.99	0.022
106. LP (2)C1 50	1072. RY (18)Sb 47	0.09	2.10	0.013
106. LP (2)C1 50	1085. RY (31)Sb 47	0.24	1.93	0.019
106. LP (2)C1 50	1091. RY (37)Sb 47	0.06	36.78	0.041
107. LP (3)C1 50	182. LV (1)Sb 47	1.85	0.34	0.022
107. LP (3)C1 50	183. LV (2)Sb 47	0.05	0.34	0.004
107. LP (3)C1 50	240. BD* (1)Sb 47-C1 51	0.91	0.38	0.017
107. LP (3)C1 50	1058. RY (4)Sb 47	0.67	0.92	0.022
107. LP (3)C1 50	1059. RY (5)Sb 47	0.08	1.56	0.010
107. LP (3)C1 50	1061. RY (7)Sb 47	0.10	1.52	0.011
107. LP (3)C1 50	1067. RY (13)Sb 47	0.21	1.58	0.016
107. LP (3)C1 50	1071. RY (17)Sb 47	0.07	2.02	0.010
107. LP (3)C1 50	1072. RY (18)Sb 47	0.13	2.13	0.015
107. LP (3)C1 50	1073. RY (19)Sb 47	0.07	2.39	0.011
107. LP (3)C1 50	1074. RY (20)Sb 47	0.09	2.19	0.013
107. LP (3)C1 50	1086. RY (32)Sb 47	0.05	33.31	0.038
107. LP (3)C1 50	1181. RY (6)C1 51	0.09	1.77	0.011
107. LP (3)C1 50	1182. RY (7)C1 51	0.05	1.39	0.008
108. LP (4)C1 50	182. LV (1)Sb 47	41.80	0.42	0.118
108. LP (4)C1 50	183. LV (2)Sb 47	5.73	0.42	0.044
108. LP (4)C1 50	240. BD* (1)Sb 47-C1 51	1.32	0.46	0.022
108. LP (4)C1 50	1055. RY (1)Sb 47	0.05	1.25	0.007
108. LP (4)C1 50	1056. RY (2)Sb 47	0.10	1.16	0.010
108. LP (4)C1 50	1057. RY (3)Sb 47	0.09	1.07	0.009
108. LP (4)C1 50	1058. RY (4)Sb 47	0.14	1.00	0.011
108. LP (4)C1 50	1059. RY (5)Sb 47	1.16	1.64	0.039
108. LP (4)C1 50	1060. RY (6)Sb 47	0.11	1.16	0.010
108. LP (4)C1 50	1061. RY (7)Sb 47	0.68	1.60	0.029
108. LP (4)C1 50	1062. RY (8)Sb 47	0.22	1.03	0.014
108. LP (4)C1 50	1063. RY (9)Sb 47	0.54	1.59	0.026
108. LP (4)C1 50	1064. RY (10)Sb 47	0.63	2.37	0.034

108. LP (4)C1 50	1065. RY (11)Sb 47	0.64	2.61	0.036
108. LP (4)C1 50	1066. RY (12)Sb 47	0.31	1.68	0.020
108. LP (4)C1 50	1067. RY (13)Sb 47	0.33	1.66	0.021
108. LP (4)C1 50	1068. RY (14)Sb 47	0.30	1.56	0.019
108. LP (4)C1 50	1070. RY (16)Sb 47	1.37	5.00	0.074
108. LP (4)C1 50	1072. RY (18)Sb 47	0.10	2.21	0.013
108. LP (4)C1 50	1073. RY (19)Sb 47	0.79	2.47	0.039
108. LP (4)C1 50	1074. RY (20)Sb 47	0.62	2.27	0.033
108. LP (4)C1 50	1075. RY (21)Sb 47	0.33	2.96	0.028
108. LP (4)C1 50	1076. RY (22)Sb 47	0.46	10.14	0.061
108. LP (4)C1 50	1078. RY (24)Sb 47	0.21	2.66	0.021
108. LP (4)C1 50	1080. RY (26)Sb 47	0.32	4.34	0.033
108. LP (4)C1 50	1081. RY (27)Sb 47	0.52	8.04	0.058
108. LP (4)C1 50	1083. RY (29)Sb 47	0.89	33.86	0.155
108. LP (4)C1 50	1084. RY (30)Sb 47	1.72	5.37	0.086
108. LP (4)C1 50	1086. RY (32)Sb 47	0.06	33.39	0.041
108. LP (4)C1 50	1087. RY (33)Sb 47	0.56	8.17	0.060
108. LP (4)C1 50	1088. RY (34)Sb 47	0.11	5.85	0.022
108. LP (4)C1 50	1089. RY (35)Sb 47	0.15	93.68	0.108
108. LP (4)C1 50	1090. RY (36)Sb 47	0.81	36.76	0.154
108. LP (4)C1 50	1091. RY (37)Sb 47	0.63	36.89	0.136
108. LP (4)C1 50	1177. RY (2)C1 51	0.06	2.55	0.011
from unit 6 to unit 4				
108. LP (4)C1 50	1096. RY (5)C1 48	0.10	1.66	0.011
108. LP (4)C1 50	1101. RY (10)C1 48	0.21	3.16	0.023
from unit 6 to unit 5				
106. LP (2)C1 50	1120. RY (1)C1 49	0.06	1.01	0.007
106. LP (2)C1 50	1127. RY (8)C1 49	0.06	2.72	0.012
within unit 6				
63. CR (2)C1 50	1157. RY (10)C1 50	2.04	18.62	0.174
63. CR (2)C1 50	1160. RY (13)C1 50	0.88	18.91	0.115
63. CR (2)C1 50	1161. RY (14)C1 50	1.43	19.58	0.149
63. CR (2)C1 50	1162. RY (15)C1 50	0.67	17.81	0.098
63. CR (2)C1 50	1171. RY (24)C1 50	1.18	18.91	0.134
63. CR (2)C1 50	1172. RY (25)C1 50	1.43	19.11	0.148
63. CR (2)C1 50	1173. RY (26)C1 50	2.67	21.80	0.215
63. CR (2)C1 50	1174. RY (27)C1 50	1.11	19.02	0.130
64. CR (3)C1 50	1155. RY (8)C1 50	1.01	10.64	0.093
64. CR (3)C1 50	1157. RY (10)C1 50	0.57	12.21	0.075
64. CR (3)C1 50	1158. RY (11)C1 50	0.97	11.41	0.094
64. CR (3)C1 50	1160. RY (13)C1 50	0.76	12.50	0.087
64. CR (3)C1 50	1163. RY (16)C1 50	0.55	10.63	0.068
64. CR (3)C1 50	1166. RY (19)C1 50	0.89	10.82	0.088
64. CR (3)C1 50	1167. RY (20)C1 50	16.21	18.08	0.483
64. CR (3)C1 50	1168. RY (21)C1 50	2.12	17.89	0.174
64. CR (3)C1 50	1169. RY (22)C1 50	3.37	17.35	0.216
65. CR (4)C1 50	1150. RY (3)C1 50	0.55	9.18	0.063
65. CR (4)C1 50	1158. RY (11)C1 50	0.71	11.41	0.080
65. CR (4)C1 50	1161. RY (14)C1 50	1.03	13.16	0.104
65. CR (4)C1 50	1164. RY (17)C1 50	2.05	11.54	0.137
65. CR (4)C1 50	1167. RY (20)C1 50	2.97	18.08	0.207
65. CR (4)C1 50	1169. RY (22)C1 50	19.75	17.35	0.523
66. CR (5)C1 50	1148. RY (1)C1 50	1.02	9.23	0.087
66. CR (5)C1 50	1154. RY (7)C1 50	1.30	9.72	0.100
66. CR (5)C1 50	1155. RY (8)C1 50	0.64	10.65	0.074
66. CR (5)C1 50	1157. RY (10)C1 50	3.22	12.21	0.177
66. CR (5)C1 50	1163. RY (16)C1 50	0.66	10.63	0.075
66. CR (5)C1 50	1167. RY (20)C1 50	1.15	18.08	0.129
66. CR (5)C1 50	1168. RY (21)C1 50	18.44	17.89	0.513
105. LP (1)C1 50	1153. RY (6)C1 50	1.07	1.86	0.040
105. LP (1)C1 50	1154. RY (7)C1 50	4.57	1.95	0.084
105. LP (1)C1 50	1155. RY (8)C1 50	3.02	2.87	0.083
105. LP (1)C1 50	1156. RY (9)C1 50	1.42	2.03	0.048
105. LP (1)C1 50	1157. RY (10)C1 50	1.01	4.44	0.060
105. LP (1)C1 50	1158. RY (11)C1 50	0.62	3.64	0.042
105. LP (1)C1 50	1160. RY (13)C1 50	0.57	4.73	0.046
105. LP (1)C1 50	1162. RY (15)C1 50	1.04	3.63	0.055
105. LP (1)C1 50	1168. RY (21)C1 50	1.00	10.11	0.090
105. LP (1)C1 50	1171. RY (24)C1 50	0.89	4.72	0.058
105. LP (1)C1 50	1172. RY (25)C1 50	1.33	4.92	0.072
105. LP (1)C1 50	1173. RY (26)C1 50	1.38	7.62	0.092
105. LP (1)C1 50	1174. RY (27)C1 50	0.65	4.84	0.050
106. LP (2)C1 50	1150. RY (3)C1 50	3.57	1.00	0.053
106. LP (2)C1 50	1153. RY (6)C1 50	3.21	1.45	0.061
106. LP (2)C1 50	1154. RY (7)C1 50	3.85	1.54	0.069
106. LP (2)C1 50	1155. RY (8)C1 50	4.02	2.46	0.089
106. LP (2)C1 50	1160. RY (13)C1 50	0.86	4.31	0.054
106. LP (2)C1 50	1163. RY (16)C1 50	0.53	2.44	0.032
106. LP (2)C1 50	1164. RY (17)C1 50	1.15	3.35	0.055
106. LP (2)C1 50	1166. RY (19)C1 50	0.57	2.63	0.035
106. LP (2)C1 50	1168. RY (21)C1 50	0.78	9.70	0.077
106. LP (2)C1 50	1169. RY (22)C1 50	3.44	9.16	0.158
107. LP (3)C1 50	1149. RY (2)C1 50	3.63	1.37	0.063
107. LP (3)C1 50	1150. RY (3)C1 50	1.53	1.03	0.035
107. LP (3)C1 50	1151. RY (4)C1 50	5.83	1.07	0.071
107. LP (3)C1 50	1152. RY (5)C1 50	4.51	1.59	0.076
107. LP (3)C1 50	1156. RY (9)C1 50	1.94	1.64	0.050
107. LP (3)C1 50	1158. RY (11)C1 50	1.38	3.26	0.060
107. LP (3)C1 50	1161. RY (14)C1 50	0.72	5.01	0.054
107. LP (3)C1 50	1164. RY (17)C1 50	0.83	3.38	0.047
107. LP (3)C1 50	1167. RY (20)C1 50	2.15	9.92	0.130
107. LP (3)C1 50	1169. RY (22)C1 50	0.97	9.20	0.084
108. LP (4)C1 50	1148. RY (1)C1 50	4.90	1.15	0.067
108. LP (4)C1 50	1149. RY (2)C1 50	1.62	1.45	0.043
108. LP (4)C1 50	1152. RY (5)C1 50	1.45	1.67	0.044
108. LP (4)C1 50	1154. RY (7)C1 50	0.83	1.65	0.033
108. LP (4)C1 50	1157. RY (10)C1 50	4.17	4.13	0.117
108. LP (4)C1 50	1167. RY (20)C1 50	1.25	10.00	0.100
108. LP (4)C1 50	1168. RY (21)C1 50	1.96	9.81	0.124

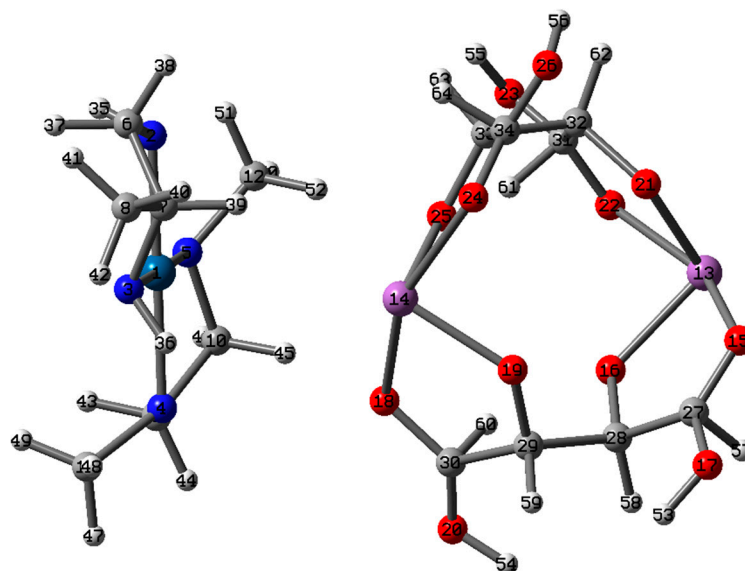
from unit 6 to unit 7					
106. LP (2)C1 50	1207. RY (4)C1 52	0.06	1.02	0.007	
106. LP (2)C1 50	1210. RY (7)C1 52	0.07	2.19	0.011	
from unit 6 to unit 8					
None above threshold					
from unit 7 to unit 1					
None above threshold					
from unit 7 to unit 2					
74. CR (3)C1 52	696. RY (3) C 21	0.06	9.71	0.022	
74. CR (3)C1 52	706. RY (13) C 21	0.08	10.97	0.026	
74. CR (3)C1 52	720. RY (1) C 22	0.07	10.47	0.024	
74. CR (3)C1 52	722. RY (3) C 22	0.16	9.70	0.035	
74. CR (3)C1 52	730. RY (11) C 22	0.09	11.87	0.029	
75. CR (4)C1 52	722. RY (3) C 22	0.11	9.70	0.029	
75. CR (4)C1 52	730. RY (11) C 22	0.06	11.87	0.024	
112. LP (1)C1 52	697. RY (4) C 21	0.08	1.77	0.011	
112. LP (1)C1 52	706. RY (13) C 21	0.11	3.22	0.017	
113. LP (2)C1 52	697. RY (4) C 21	0.07	1.34	0.008	
113. LP (2)C1 52	720. RY (1) C 22	0.06	2.29	0.011	
113. LP (2)C1 52	722. RY (3) C 22	0.06	1.52	0.008	
113. LP (2)C1 52	729. RY (10) C 22	0.07	3.21	0.013	
114. LP (3)C1 52	217. BD* (2) C 21- C 22	0.07	0.21	0.003	
114. LP (3)C1 52	611. RY (1) C 17	0.05	2.45	0.010	
114. LP (3)C1 52	671. RY (4) C 20	0.06	1.51	0.009	
114. LP (3)C1 52	697. RY (4) C 21	0.35	1.34	0.019	
114. LP (3)C1 52	704. RY (11) C 21	0.06	2.68	0.011	
114. LP (3)C1 52	706. RY (13) C 21	0.38	2.79	0.029	
114. LP (3)C1 52	720. RY (1) C 22	0.09	2.29	0.013	
114. LP (3)C1 52	722. RY (3) C 22	0.60	1.52	0.027	
114. LP (3)C1 52	729. RY (10) C 22	0.10	3.21	0.016	
114. LP (3)C1 52	730. RY (11) C 22	0.44	3.69	0.036	
114. LP (3)C1 52	732. RY (13) C 22	0.08	3.19	0.015	
115. LP (4)C1 52	217. BD* (2) C 21- C 22	0.08	0.30	0.005	
115. LP (4)C1 52	696. RY (3) C 21	0.08	1.62	0.010	
115. LP (4)C1 52	706. RY (13) C 21	0.08	2.89	0.014	
115. LP (4)C1 52	722. RY (3) C 22	0.14	1.62	0.013	
115. LP (4)C1 52	730. RY (11) C 22	0.06	3.79	0.013	
from unit 7 to unit 3					
73. CR (2)C1 52	183. LV (2)Sb 47	0.25	14.99	0.055	
73. CR (2)C1 52	1056. RY (2)Sb 47	0.22	15.73	0.053	
73. CR (2)C1 52	1057. RY (3)Sb 47	0.09	15.64	0.033	
73. CR (2)C1 52	1064. RY (10)Sb 47	0.09	16.94	0.035	
74. CR (3)C1 52	1055. RY (1)Sb 47	0.08	9.31	0.025	
74. CR (3)C1 52	1056. RY (2)Sb 47	0.09	9.23	0.025	
74. CR (3)C1 52	1064. RY (10)Sb 47	0.10	10.43	0.028	
74. CR (3)C1 52	1074. RY (20)Sb 47	0.05	10.34	0.021	
74. CR (3)C1 52	1084. RY (30)Sb 47	0.06	13.43	0.026	
75. CR (4)C1 52	183. LV (2)Sb 47	0.12	8.49	0.028	
75. CR (4)C1 52	1056. RY (2)Sb 47	0.18	9.23	0.036	
75. CR (4)C1 52	1064. RY (10)Sb 47	0.24	10.43	0.045	
75. CR (4)C1 52	1069. RY (15)Sb 47	0.07	9.58	0.023	
75. CR (4)C1 52	1070. RY (16)Sb 47	0.12	13.07	0.035	
75. CR (4)C1 52	1074. RY (20)Sb 47	0.07	10.34	0.025	
75. CR (4)C1 52	1078. RY (24)Sb 47	0.06	10.72	0.023	
75. CR (4)C1 52	1084. RY (30)Sb 47	0.13	13.44	0.038	
76. CR (5)C1 52	1058. RY (4)Sb 47	0.10	9.06	0.027	
112. LP (1)C1 52	182. LV (1)Sb 47	1.28	0.74	0.027	
112. LP (1)C1 52	183. LV (2)Sb 47	7.01	0.74	0.064	
112. LP (1)C1 52	240. BD* (1)Sb 47-C1 51	0.11	0.78	0.008	
112. LP (1)C1 52	1057. RY (3)Sb 47	0.28	1.39	0.018	
112. LP (1)C1 52	1069. RY (15)Sb 47	0.15	1.83	0.015	
112. LP (1)C1 52	1071. RY (17)Sb 47	0.42	2.42	0.028	
112. LP (1)C1 52	1072. RY (18)Sb 47	0.19	2.53	0.020	
112. LP (1)C1 52	1073. RY (19)Sb 47	0.11	2.79	0.016	
112. LP (1)C1 52	1076. RY (22)Sb 47	0.13	10.46	0.033	
112. LP (1)C1 52	1091. RY (37)Sb 47	0.10	37.21	0.054	
113. LP (2)C1 52	182. LV (1)Sb 47	0.72	0.30	0.013	
113. LP (2)C1 52	183. LV (2)Sb 47	1.27	0.30	0.018	
113. LP (2)C1 52	240. BD* (1)Sb 47-C1 51	0.06	0.35	0.004	
113. LP (2)C1 52	1057. RY (3)Sb 47	0.09	0.96	0.008	
113. LP (2)C1 52	1058. RY (4)Sb 47	0.20	0.89	0.012	
113. LP (2)C1 52	1063. RY (9)Sb 47	0.13	1.48	0.012	
113. LP (2)C1 52	1068. RY (14)Sb 47	0.08	1.45	0.010	
113. LP (2)C1 52	1073. RY (19)Sb 47	0.14	2.36	0.016	
113. LP (2)C1 52	1079. RY (25)Sb 47	0.08	2.79	0.014	
113. LP (2)C1 52	1082. RY (28)Sb 47	0.05	2.44	0.010	
113. LP (2)C1 52	1085. RY (31)Sb 47	0.13	1.93	0.014	
113. LP (2)C1 52	1090. RY (36)Sb 47	0.06	36.65	0.043	
114. LP (3)C1 52	182. LV (1)Sb 47	0.31	0.30	0.009	
114. LP (3)C1 52	240. BD* (1)Sb 47-C1 51	0.97	0.35	0.016	
114. LP (3)C1 52	1056. RY (2)Sb 47	0.06	1.05	0.007	
114. LP (3)C1 52	1057. RY (3)Sb 47	0.24	0.96	0.014	
114. LP (3)C1 52	1059. RY (5)Sb 47	0.15	1.52	0.014	
114. LP (3)C1 52	1060. RY (6)Sb 47	0.06	1.04	0.007	
114. LP (3)C1 52	1066. RY (12)Sb 47	0.18	1.56	0.015	
114. LP (3)C1 52	1072. RY (18)Sb 47	0.13	2.09	0.015	
114. LP (3)C1 52	1075. RY (21)Sb 47	0.28	2.84	0.025	
114. LP (3)C1 52	1181. RY (6)C1 51	0.08	1.73	0.011	
115. LP (4)C1 52	182. LV (1)Sb 47	6.17	0.40	0.044	
115. LP (4)C1 52	183. LV (2)Sb 47	40.10	0.40	0.113	
115. LP (4)C1 52	240. BD* (1)Sb 47-C1 51	1.85	0.44	0.026	
115. LP (4)C1 52	1055. RY (1)Sb 47	0.09	1.23	0.009	
115. LP (4)C1 52	1056. RY (2)Sb 47	0.42	1.14	0.020	
115. LP (4)C1 52	1058. RY (4)Sb 47	0.06	0.98	0.007	
115. LP (4)C1 52	1059. RY (5)Sb 47	0.89	1.62	0.034	
115. LP (4)C1 52	1060. RY (6)Sb 47	0.12	1.14	0.010	
115. LP (4)C1 52	1061. RY (7)Sb 47	0.89	1.58	0.033	
115. LP (4)C1 52	1062. RY (8)Sb 47	0.26	1.01	0.014	
115. LP (4)C1 52	1064. RY (10)Sb 47	0.33	2.35	0.025	

115. LP (4)C1 52	1065. RY (11)Sb 47	1.04	2.59	0.046
115. LP (4)C1 52	1066. RY (12)Sb 47	0.57	1.66	0.027
115. LP (4)C1 52	1067. RY (13)Sb 47	0.26	1.64	0.019
115. LP (4)C1 52	1070. RY (16)Sb 47	1.01	4.98	0.063
115. LP (4)C1 52	1071. RY (17)Sb 47	0.39	2.08	0.025
115. LP (4)C1 52	1072. RY (18)Sb 47	0.15	2.19	0.016
115. LP (4)C1 52	1073. RY (19)Sb 47	0.09	2.45	0.013
115. LP (4)C1 52	1074. RY (20)Sb 47	0.07	2.25	0.011
115. LP (4)C1 52	1075. RY (21)Sb 47	0.23	2.94	0.023
115. LP (4)C1 52	1076. RY (22)Sb 47	0.16	10.12	0.036
115. LP (4)C1 52	1077. RY (23)Sb 47	0.09	2.04	0.012
115. LP (4)C1 52	1078. RY (24)Sb 47	0.25	2.64	0.023
115. LP (4)C1 52	1079. RY (25)Sb 47	0.27	2.89	0.025
115. LP (4)C1 52	1080. RY (26)Sb 47	0.52	4.32	0.042
115. LP (4)C1 52	1081. RY (27)Sb 47	0.46	8.02	0.054
115. LP (4)C1 52	1083. RY (29)Sb 47	1.14	33.84	0.175
115. LP (4)C1 52	1084. RY (30)Sb 47	0.08	5.35	0.018
115. LP (4)C1 52	1085. RY (31)Sb 47	0.13	2.03	0.015
115. LP (4)C1 52	1087. RY (33)Sb 47	0.28	8.15	0.042
115. LP (4)C1 52	1088. RY (34)Sb 47	0.43	5.84	0.045
115. LP (4)C1 52	1089. RY (35)Sb 47	0.28	93.66	0.144
115. LP (4)C1 52	1090. RY (36)Sb 47	0.40	36.74	0.108
115. LP (4)C1 52	1091. RY (37)Sb 47	0.64	36.87	0.137
from unit 7 to unit 4				
None above threshold				
from unit 7 to unit 5				
115. LP (4)C1 52	1124. RY (5)C1 49	0.12	2.15	0.014
115. LP (4)C1 52	1129. RY (10)C1 49	0.06	2.68	0.012
115. LP (4)C1 52	1130. RY (11)C1 49	0.16	4.04	0.022
from unit 7 to unit 6				
None above threshold				
within unit 7				
72. CR (1)C1 52	1227. RY (24)C1 52	0.98	115.72	0.300
73. CR (2)C1 52	1214. RY (11)C1 52	2.23	18.91	0.183
73. CR (2)C1 52	1217. RY (14)C1 52	0.64	18.45	0.097
73. CR (2)C1 52	1227. RY (24)C1 52	5.08	28.60	0.340
73. CR (2)C1 52	1228. RY (25)C1 52	0.86	18.69	0.113
74. CR (3)C1 52	1208. RY (5)C1 52	0.58	10.67	0.070
74. CR (3)C1 52	1213. RY (10)C1 52	1.05	11.14	0.097
74. CR (3)C1 52	1214. RY (11)C1 52	0.57	12.40	0.075
74. CR (3)C1 52	1216. RY (13)C1 52	0.74	11.59	0.082
74. CR (3)C1 52	1218. RY (15)C1 52	0.54	11.12	0.069
74. CR (3)C1 52	1222. RY (19)C1 52	12.61	17.72	0.422
74. CR (3)C1 52	1223. RY (20)C1 52	8.08	17.29	0.334
74. CR (3)C1 52	1224. RY (21)C1 52	0.96	17.76	0.116
74. CR (3)C1 52	1227. RY (24)C1 52	0.73	22.10	0.113
75. CR (4)C1 52	1204. RY (1)C1 52	0.80	9.25	0.077
75. CR (4)C1 52	1210. RY (7)C1 52	1.07	10.37	0.094
75. CR (4)C1 52	1213. RY (10)C1 52	0.88	11.14	0.089
75. CR (4)C1 52	1214. RY (11)C1 52	0.88	12.41	0.093
75. CR (4)C1 52	1218. RY (15)C1 52	1.96	11.13	0.132
75. CR (4)C1 52	1222. RY (19)C1 52	3.49	17.72	0.222
75. CR (4)C1 52	1224. RY (21)C1 52	15.59	17.76	0.470
75. CR (4)C1 52	1225. RY (22)C1 52	2.16	11.28	0.139
76. CR (5)C1 52	1207. RY (4)C1 52	0.61	9.19	0.067
76. CR (5)C1 52	1209. RY (6)C1 52	0.63	9.53	0.069
76. CR (5)C1 52	1216. RY (13)C1 52	0.51	11.59	0.069
76. CR (5)C1 52	1217. RY (14)C1 52	1.61	11.95	0.124
76. CR (5)C1 52	1219. RY (16)C1 52	0.59	10.44	0.070
76. CR (5)C1 52	1222. RY (19)C1 52	5.37	17.72	0.275
76. CR (5)C1 52	1223. RY (20)C1 52	14.30	17.29	0.444
76. CR (5)C1 52	1224. RY (21)C1 52	3.40	17.76	0.219
112. LP (1)C1 52	1210. RY (7)C1 52	6.19	2.62	0.114
112. LP (1)C1 52	1211. RY (8)C1 52	1.41	2.05	0.048
112. LP (1)C1 52	1213. RY (10)C1 52	0.58	3.39	0.040
112. LP (1)C1 52	1214. RY (11)C1 52	1.24	4.66	0.068
112. LP (1)C1 52	1217. RY (14)C1 52	0.85	4.20	0.053
112. LP (1)C1 52	1221. RY (18)C1 52	0.50	3.35	0.037
112. LP (1)C1 52	1224. RY (21)C1 52	0.82	10.01	0.081
112. LP (1)C1 52	1227. RY (24)C1 52	1.89	14.35	0.147
112. LP (1)C1 52	1228. RY (25)C1 52	0.64	4.43	0.048
113. LP (2)C1 52	1206. RY (3)C1 52	2.31	1.03	0.044
113. LP (2)C1 52	1207. RY (4)C1 52	2.79	1.02	0.048
113. LP (2)C1 52	1208. RY (5)C1 52	0.87	2.49	0.042
113. LP (2)C1 52	1209. RY (6)C1 52	7.18	1.35	0.088
113. LP (2)C1 52	1211. RY (8)C1 52	2.58	1.61	0.058
113. LP (2)C1 52	1212. RY (9)C1 52	1.00	1.56	0.035
113. LP (2)C1 52	1216. RY (13)C1 52	1.43	3.41	0.062
113. LP (2)C1 52	1217. RY (14)C1 52	1.32	3.77	0.063
113. LP (2)C1 52	1219. RY (16)C1 52	0.86	2.27	0.039
113. LP (2)C1 52	1223. RY (20)C1 52	4.06	9.11	0.172
114. LP (3)C1 52	1205. RY (2)C1 52	1.96	1.75	0.052
114. LP (3)C1 52	1206. RY (3)C1 52	1.56	1.03	0.036
114. LP (3)C1 52	1207. RY (4)C1 52	3.33	1.01	0.052
114. LP (3)C1 52	1208. RY (5)C1 52	2.53	2.49	0.071
114. LP (3)C1 52	1211. RY (8)C1 52	2.64	1.61	0.058
114. LP (3)C1 52	1218. RY (15)C1 52	2.32	2.94	0.074
114. LP (3)C1 52	1222. RY (19)C1 52	3.99	9.54	0.174
115. LP (4)C1 52	1204. RY (1)C1 52	5.01	1.16	0.068
115. LP (4)C1 52	1205. RY (2)C1 52	0.85	1.84	0.035
115. LP (4)C1 52	1208. RY (5)C1 52	0.98	2.59	0.045
115. LP (4)C1 52	1210. RY (7)C1 52	1.14	2.28	0.045
115. LP (4)C1 52	1213. RY (10)C1 52	1.98	3.05	0.069
115. LP (4)C1 52	1214. RY (11)C1 52	2.27	4.32	0.088
115. LP (4)C1 52	1224. RY (21)C1 52	2.90	9.67	0.150
115. LP (4)C1 52	1225. RY (22)C1 52	0.80	3.19	0.045
from unit 7 to unit 8				
None above threshold				

from unit 8 to unit 1						
None above threshold						
from unit 8 to unit 2						
174. BD (1) N 53- C 54	808. RY (1) C 27	0.06	2.94	0.012		
176. BD (3) N 53- C 54	808. RY (1) C 27	0.10	2.27	0.013		
from unit 8 to unit 3						
None above threshold						
from unit 8 to unit 4						
None above threshold						
from unit 8 to unit 5						
None above threshold						
from unit 8 to unit 6						
None above threshold						
from unit 8 to unit 7						
None above threshold						
within unit 8						
77. CR (1) N 53	241. BD* (1) N 53- C 54	1.81	16.83	0.156		
77. CR (1) N 53	1242. RY (11) N 53	7.59	25.81	0.395		
77. CR (1) N 53	1243. RY (12) N 53	13.06	29.42	0.553		
77. CR (1) N 53	1244. RY (13) N 53	3.80	20.85	0.251		
77. CR (1) N 53	1245. RY (14) N 53	2.87	20.63	0.217		
77. CR (1) N 53	1246. RY (15) N 53	3.04	21.90	0.231		
77. CR (1) N 53	1247. RY (16) N 53	1.23	19.56	0.138		
77. CR (1) N 53	1250. RY (19) N 53	0.81	20.76	0.115		
77. CR (1) N 53	1257. RY (26) N 53	3.53	22.29	0.250		
78. CR (1) C 54	241. BD* (1) N 53- C 54	1.11	12.41	0.105		
78. CR (1) C 54	244. BD* (1) C 54- C 55	1.48	11.87	0.118		
78. CR (1) C 54	1258. RY (1) C 54	0.51	12.70	0.071		
78. CR (1) C 54	1270. RY (13) C 54	1.74	15.11	0.145		
78. CR (1) C 54	1271. RY (14) C 54	0.72	14.46	0.091		
78. CR (1) C 54	1272. RY (15) C 54	3.36	14.86	0.199		
78. CR (1) C 54	1273. RY (16) C 54	1.93	14.04	0.147		
78. CR (1) C 54	1280. RY (23) C 54	2.02	15.35	0.157		
78. CR (1) C 54	1281. RY (24) C 54	1.11	14.98	0.115		
78. CR (1) C 54	1282. RY (25) C 54	19.27	25.73	0.628		
79. CR (1) C 55	244. BD* (1) C 54- C 55	0.98	11.85	0.096		
79. CR (1) C 55	245. BD* (1) C 55- H 56	0.67	12.05	0.080		
79. CR (1) C 55	246. BD* (1) C 55- H 57	0.67	12.04	0.080		
79. CR (1) C 55	247. BD* (1) C 55- H 58	0.67	12.05	0.080		
79. CR (1) C 55	1264. RY (7) C 54	0.89	13.42	0.097		
79. CR (1) C 55	1269. RY (12) C 54	1.07	13.60	0.108		
79. CR (1) C 55	1287. RY (4) C 55	0.91	12.87	0.096		
79. CR (1) C 55	1288. RY (5) C 55	0.93	13.82	0.101		
79. CR (1) C 55	1289. RY (6) C 55	3.90	14.31	0.211		
79. CR (1) C 55	1290. RY (7) C 55	6.72	14.66	0.280		
79. CR (1) C 55	1291. RY (8) C 55	1.19	13.94	0.115		
79. CR (1) C 55	1292. RY (9) C 55	0.98	15.22	0.109		
79. CR (1) C 55	1296. RY (13) C 55	4.28	16.74	0.239		
79. CR (1) C 55	1297. RY (14) C 55	0.83	13.86	0.096		
79. CR (1) C 55	1298. RY (15) C 55	5.50	17.58	0.278		
79. CR (1) C 55	1300. RY (17) C 55	9.32	18.16	0.367		
79. CR (1) C 55	1301. RY (18) C 55	2.25	14.41	0.161		
79. CR (1) C 55	1303. RY (20) C 55	1.61	14.60	0.137		
79. CR (1) C 55	1315. RY (1) H 57	0.50	12.88	0.072		
116. LP (1) N 53	241. BD* (1) N 53- C 54	2.41	1.35	0.051		
116. LP (1) N 53	244. BD* (1) C 54- C 55	4.90	0.82	0.056		
116. LP (1) N 53	1232. RY (1) N 53	4.87	2.54	0.099		
116. LP (1) N 53	1233. RY (2) N 53	2.46	1.41	0.053		
116. LP (1) N 53	1234. RY (3) N 53	0.51	1.43	0.024		
116. LP (1) N 53	1235. RY (4) N 53	21.92	1.57	0.165		
116. LP (1) N 53	1238. RY (7) N 53	1.01	3.11	0.050		
116. LP (1) N 53	1243. RY (12) N 53	1.13	13.95	0.112		
116. LP (1) N 53	1244. RY (13) N 53	0.82	5.38	0.059		
116. LP (1) N 53	1258. RY (1) C 54	9.10	1.64	0.109		
116. LP (1) N 53	1262. RY (5) C 54	0.96	3.29	0.050		
116. LP (1) N 53	1263. RY (6) C 54	0.52	2.45	0.032		
174. BD (1) N 53- C 54	241. BD* (1) N 53- C 54	1.31	1.92	0.045		
174. BD (1) N 53- C 54	244. BD* (1) C 54- C 55	2.76	1.39	0.055		
174. BD (1) N 53- C 54	1235. RY (4) N 53	0.56	2.14	0.031		
174. BD (1) N 53- C 54	1243. RY (12) N 53	1.05	14.52	0.110		
174. BD (1) N 53- C 54	1244. RY (13) N 53	0.70	5.95	0.058		
174. BD (1) N 53- C 54	1246. RY (15) N 53	0.64	7.00	0.060		
174. BD (1) N 53- C 54	1258. RY (1) C 54	4.34	2.21	0.087		
174. BD (1) N 53- C 54	1282. RY (25) C 54	1.14	15.24	0.117		
174. BD (1) N 53- C 54	1286. RY (3) C 55	0.90	3.63	0.051		
175. BD (2) N 53- C 54	242. BD* (2) N 53- C 54	4.37	0.44	0.039		
175. BD (2) N 53- C 54	245. BD* (1) C 55- H 56	1.34	0.92	0.031		
175. BD (2) N 53- C 54	246. BD* (1) C 55- H 57	0.60	0.91	0.021		
175. BD (2) N 53- C 54	1233. RY (2) N 53	4.84	1.31	0.071		
175. BD (2) N 53- C 54	1234. RY (3) N 53	6.39	1.33	0.082		
175. BD (2) N 53- C 54	1236. RY (5) N 53	0.95	1.96	0.039		
175. BD (2) N 53- C 54	1260. RY (3) C 54	2.17	1.95	0.058		
175. BD (2) N 53- C 54	1263. RY (6) C 54	0.68	2.35	0.036		
175. BD (2) N 53- C 54	1265. RY (8) C 54	1.55	2.69	0.058		
175. BD (2) N 53- C 54	1266. RY (9) C 54	1.15	2.40	0.047		
176. BD (3) N 53- C 54	243. BD* (3) N 53- C 54	4.40	0.44	0.039		
176. BD (3) N 53- C 54	246. BD* (1) C 55- H 57	0.82	0.91	0.024		
176. BD (3) N 53- C 54	247. BD* (1) C 55- H 58	1.25	0.92	0.030		
176. BD (3) N 53- C 54	1233. RY (2) N 53	5.80	1.31	0.078		
176. BD (3) N 53- C 54	1234. RY (3) N 53	5.95	1.33	0.079		
176. BD (3) N 53- C 54	1235. RY (4) N 53	1.03	1.47	0.035		
176. BD (3) N 53- C 54	1259. RY (2) C 54	2.58	1.89	0.062		
176. BD (3) N 53- C 54	1262. RY (5) C 54	0.80	3.20	0.045		
176. BD (3) N 53- C 54	1263. RY (6) C 54	1.35	2.35	0.050		
176. BD (3) N 53- C 54	1264. RY (7) C 54	0.98	2.28	0.042		

177. BD (1) C 54- C 55	241. BD* (1) N 53- C 54	0.78	1.55	0.031
177. BD (1) C 54- C 55	1232. RY (1) N 53	3.41	2.73	0.086
177. BD (1) C 54- C 55	1240. RY (9) N 53	0.54	5.29	0.048
177. BD (1) C 54- C 55	1261. RY (4) C 54	1.60	3.73	0.069
177. BD (1) C 54- C 55	1272. RY (15) C 54	0.77	3.99	0.049
177. BD (1) C 54- C 55	1282. RY (25) C 54	1.33	14.87	0.125
177. BD (1) C 54- C 55	1286. RY (3) C 55	0.96	3.26	0.050
177. BD (1) C 54- C 55	1287. RY (4) C 55	2.68	2.03	0.066
177. BD (1) C 54- C 55	1298. RY (15) C 55	0.54	6.75	0.054
178. BD (1) C 55- H 56	241. BD* (1) N 53- C 54	2.36	1.44	0.052
178. BD (1) C 55- H 56	242. BD* (2) N 53- C 54	3.96	0.63	0.044
178. BD (1) C 55- H 56	245. BD* (1) C 55- H 56	1.48	1.10	0.036
178. BD (1) C 55- H 56	1260. RY (3) C 54	1.26	2.13	0.046
178. BD (1) C 55- H 56	1285. RY (2) C 55	2.24	1.58	0.053
178. BD (1) C 55- H 56	1289. RY (6) C 55	0.79	3.36	0.046
178. BD (1) C 55- H 56	1290. RY (7) C 55	1.50	3.70	0.067
178. BD (1) C 55- H 56	1291. RY (8) C 55	0.58	2.99	0.037
178. BD (1) C 55- H 56	1300. RY (17) C 55	1.21	7.21	0.083
178. BD (1) C 55- H 56	1310. RY (1) H 56	2.82	2.15	0.070
178. BD (1) C 55- H 56	1311. RY (2) H 56	1.03	2.22	0.043
178. BD (1) C 55- H 56	1313. RY (4) H 56	0.55	3.07	0.037
179. BD (1) C 55- H 57	241. BD* (1) N 53- C 54	2.26	1.44	0.051
179. BD (1) C 55- H 57	242. BD* (2) N 53- C 54	1.85	0.63	0.030
179. BD (1) C 55- H 57	243. BD* (3) N 53- C 54	2.52	0.63	0.036
179. BD (1) C 55- H 57	246. BD* (1) C 55- H 57	1.61	1.09	0.037
179. BD (1) C 55- H 57	1259. RY (2) C 54	1.05	2.07	0.042
179. BD (1) C 55- H 57	1284. RY (1) C 55	1.56	1.62	0.045
179. BD (1) C 55- H 57	1289. RY (6) C 55	1.12	3.37	0.055
179. BD (1) C 55- H 57	1296. RY (13) C 55	0.68	5.79	0.056
179. BD (1) C 55- H 57	1299. RY (16) C 55	0.59	2.87	0.037
179. BD (1) C 55- H 57	1300. RY (17) C 55	0.63	7.21	0.060
179. BD (1) C 55- H 57	1302. RY (19) C 55	0.56	2.21	0.032
179. BD (1) C 55- H 57	1304. RY (21) C 55	0.85	3.42	0.048
179. BD (1) C 55- H 57	1315. RY (1) H 57	2.74	1.93	0.065
179. BD (1) C 55- H 57	1316. RY (2) H 57	0.58	2.64	0.035
179. BD (1) C 55- H 57	1318. RY (4) H 57	1.25	2.98	0.054
180. BD (1) C 55- H 58	241. BD* (1) N 53- C 54	2.39	1.44	0.052
180. BD (1) C 55- H 58	243. BD* (3) N 53- C 54	3.58	0.63	0.042
180. BD (1) C 55- H 58	247. BD* (1) C 55- H 58	1.51	1.10	0.036
180. BD (1) C 55- H 58	1259. RY (2) C 54	0.93	2.07	0.039
180. BD (1) C 55- H 58	1284. RY (1) C 55	1.41	1.61	0.043
180. BD (1) C 55- H 58	1285. RY (2) C 55	0.51	1.58	0.025
180. BD (1) C 55- H 58	1289. RY (6) C 55	0.66	3.36	0.042
180. BD (1) C 55- H 58	1290. RY (7) C 55	2.26	3.70	0.082
180. BD (1) C 55- H 58	1291. RY (8) C 55	0.78	2.99	0.043
180. BD (1) C 55- H 58	1301. RY (18) C 55	1.50	3.46	0.064
180. BD (1) C 55- H 58	1320. RY (1) H 58	3.00	2.20	0.073
180. BD (1) C 55- H 58	1321. RY (2) H 58	0.78	2.15	0.036
180. BD (1) C 55- H 58	1323. RY (4) H 58	0.57	3.11	0.038

2.2 PEPTAS



SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
=====				
from unit 1 to unit 2				
54. LP (1)Pt 1	191. BD* (1)Sb 14- O 25	0.06	0.57	0.005
54. LP (1)Pt 1	587. RY (13)Sb 14	0.11	2.05	0.014
55. LP (2)Pt 1	190. BD* (1)Sb 14- O 19	0.08	0.45	0.005
55. LP (2)Pt 1	575. RY (1)Sb 14	0.55	1.80	0.028
55. LP (2)Pt 1	576. RY (2)Sb 14	0.06	1.98	0.010
55. LP (2)Pt 1	577. RY (3)Sb 14	0.32	1.85	0.022

55.	LP	(2)Pt	1	578.	RY	(4)Sb	14	0.88	1.33	0.031
55.	LP	(2)Pt	1	581.	RY	(7)Sb	14	0.25	1.69	0.018
55.	LP	(2)Pt	1	585.	RY	(11)Sb	14	2.09	1.61	0.052
55.	LP	(2)Pt	1	586.	RY	(12)Sb	14	0.54	1.98	0.029
55.	LP	(2)Pt	1	587.	RY	(13)Sb	14	8.69	1.95	0.116
55.	LP	(2)Pt	1	588.	RY	(14)Sb	14	0.16	1.62	0.014
55.	LP	(2)Pt	1	589.	RY	(15)Sb	14	1.84	1.60	0.048
55.	LP	(2)Pt	1	590.	RY	(16)Sb	14	0.95	2.16	0.040
55.	LP	(2)Pt	1	591.	RY	(17)Sb	14	0.24	2.18	0.021
55.	LP	(2)Pt	1	592.	RY	(18)Sb	14	0.06	1.67	0.009
55.	LP	(2)Pt	1	594.	RY	(20)Sb	14	0.16	2.74	0.019
55.	LP	(2)Pt	1	595.	RY	(21)Sb	14	0.06	1.99	0.010
55.	LP	(2)Pt	1	596.	RY	(22)Sb	14	0.30	2.29	0.023
55.	LP	(2)Pt	1	597.	RY	(23)Sb	14	0.55	2.19	0.031
55.	LP	(2)Pt	1	598.	RY	(24)Sb	14	0.06	2.30	0.011
55.	LP	(2)Pt	1	599.	RY	(25)Sb	14	0.20	3.00	0.022
55.	LP	(2)Pt	1	601.	RY	(27)Sb	14	0.09	3.23	0.016
55.	LP	(2)Pt	1	602.	RY	(28)Sb	14	0.15	4.72	0.024
55.	LP	(2)Pt	1	603.	RY	(29)Sb	14	0.22	7.31	0.035
55.	LP	(2)Pt	1	604.	RY	(30)Sb	14	0.21	14.38	0.049
55.	LP	(2)Pt	1	691.	RY	(2) O	18	0.47	1.64	0.025
55.	LP	(2)Pt	1	692.	RY	(3) O	18	0.09	1.50	0.010
55.	LP	(2)Pt	1	694.	RY	(5) O	18	0.20	2.16	0.019
55.	LP	(2)Pt	1	697.	RY	(8) O	18	0.05	2.72	0.011
55.	LP	(2)Pt	1	698.	RY	(9) O	18	0.09	2.76	0.014
55.	LP	(2)Pt	1	718.	RY	(3) O	19	0.06	1.72	0.009
55.	LP	(2)Pt	1	719.	RY	(4) O	19	0.28	1.80	0.020
55.	LP	(2)Pt	1	721.	RY	(6) O	19	0.08	2.99	0.013
55.	LP	(2)Pt	1	743.	RY	(2) O	20	0.06	1.54	0.008
55.	LP	(2)Pt	1	847.	RY	(2) O	24	0.07	1.56	0.010
55.	LP	(2)Pt	1	848.	RY	(3) O	24	0.08	1.56	0.010
55.	LP	(2)Pt	1	850.	RY	(5) O	24	0.20	2.19	0.019
55.	LP	(2)Pt	1	874.	RY	(3) O	25	0.07	1.84	0.010
55.	LP	(2)Pt	1	979.	RY	(4) C	29	0.23	1.89	0.018
55.	LP	(2)Pt	1	982.	RY	(7) C	29	0.07	2.15	0.011
55.	LP	(2)Pt	1	985.	RY	(10) C	29	0.09	4.01	0.016
55.	LP	(2)Pt	1	1008.	RY	(7) C	30	0.05	2.39	0.010
55.	LP	(2)Pt	1	1010.	RY	(9) C	30	0.51	2.74	0.033
55.	LP	(2)Pt	1	1011.	RY	(10) C	30	0.06	2.26	0.010
55.	LP	(2)Pt	1	1012.	RY	(11) C	30	0.18	2.82	0.020
55.	LP	(2)Pt	1	1013.	RY	(12) C	30	0.51	2.17	0.030
55.	LP	(2)Pt	1	1016.	RY	(15) C	30	0.06	2.99	0.012
55.	LP	(2)Pt	1	1017.	RY	(16) C	30	0.05	3.08	0.011
55.	LP	(2)Pt	1	1037.	RY	(10) C	31	0.09	2.09	0.012
55.	LP	(2)Pt	1	1057.	RY	(4) C	32	0.09	1.94	0.012
55.	LP	(2)Pt	1	1063.	RY	(10) C	32	0.05	3.81	0.013
55.	LP	(2)Pt	1	1070.	RY	(17) C	32	0.10	3.02	0.016
55.	LP	(2)Pt	1	1080.	RY	(1) C	33	0.08	1.41	0.010
55.	LP	(2)Pt	1	1085.	RY	(6) C	33	0.35	2.22	0.025
55.	LP	(2)Pt	1	1088.	RY	(9) C	33	0.16	2.76	0.019
55.	LP	(2)Pt	1	1089.	RY	(10) C	33	0.07	2.55	0.012
55.	LP	(2)Pt	1	1092.	RY	(13) C	33	0.07	3.72	0.015
55.	LP	(2)Pt	1	1108.	RY	(3) C	34	0.12	2.17	0.015
55.	LP	(2)Pt	1	1109.	RY	(4) C	34	0.08	1.63	0.010
55.	LP	(2)Pt	1	1113.	RY	(8) C	34	0.39	2.55	0.028
55.	LP	(2)Pt	1	1115.	RY	(10) C	34	0.19	2.69	0.020
55.	LP	(2)Pt	1	1120.	RY	(15) C	34	0.11	2.49	0.015
55.	LP	(2)Pt	1	1252.	RY	(1) H	59	0.10	1.22	0.010
55.	LP	(2)Pt	1	1272.	RY	(1) H	63	0.81	1.57	0.032
55.	LP	(2)Pt	1	1273.	RY	(2) H	63	0.06	2.75	0.011
55.	LP	(2)Pt	1	1274.	RY	(3) H	63	0.05	2.67	0.011
55.	LP	(2)Pt	1	1275.	RY	(4) H	63	0.07	2.78	0.012
55.	LP	(2)Pt	1	1276.	RY	(5) H	63	0.11	3.06	0.016
55.	LP	(2)Pt	1	1277.	RY	(1) H	64	0.16	1.47	0.014
57.	LP	(1) N	2	578.	RY	(4)Sb	14	0.07	1.45	0.009
57.	LP	(1) N	2	585.	RY	(11)Sb	14	0.15	1.74	0.014
57.	LP	(1) N	2	587.	RY	(13)Sb	14	0.38	2.08	0.025
57.	LP	(1) N	2	589.	RY	(15)Sb	14	0.10	1.73	0.011
58.	LP	(1) N	3	190.	BD*	(1)Sb	14- O 19	0.06	0.58	0.005
58.	LP	(1) N	3	578.	RY	(4)Sb	14	0.09	1.45	0.010
58.	LP	(1) N	3	585.	RY	(11)Sb	14	0.13	1.74	0.013
58.	LP	(1) N	3	587.	RY	(13)Sb	14	0.45	2.07	0.027
58.	LP	(1) N	3	589.	RY	(15)Sb	14	0.06	1.72	0.009
59.	LP	(1) N	4	585.	RY	(11)Sb	14	0.18	1.78	0.016
59.	LP	(1) N	4	587.	RY	(13)Sb	14	0.79	2.12	0.036
59.	LP	(1) N	4	589.	RY	(15)Sb	14	0.18	1.77	0.016
59.	LP	(1) N	4	590.	RY	(16)Sb	14	0.10	2.33	0.014
59.	LP	(1) N	4	691.	RY	(2) O	18	0.05	1.81	0.009
59.	LP	(1) N	4	1010.	RY	(9) C	30	0.06	2.90	0.012
59.	LP	(1) N	4	1272.	RY	(1) H	63	0.08	1.74	0.011
60.	LP	(1) N	5	575.	RY	(1)Sb	14	0.08	1.95	0.011
60.	LP	(1) N	5	578.	RY	(4)Sb	14	0.16	1.48	0.014
60.	LP	(1) N	5	585.	RY	(11)Sb	14	0.23	1.76	0.018
60.	LP	(1) N	5	587.	RY	(13)Sb	14	1.07	2.10	0.042
60.	LP	(1) N	5	589.	RY	(15)Sb	14	0.21	1.75	0.017
60.	LP	(1) N	5	590.	RY	(16)Sb	14	0.11	2.31	0.014
60.	LP	(1) N	5	596.	RY	(22)Sb	14	0.06	2.44	0.011
60.	LP	(1) N	5	597.	RY	(23)Sb	14	0.06	2.34	0.011
60.	LP	(1) N	5	1010.	RY	(9) C	30	0.05	2.89	0.011
60.	LP	(1) N	5	1013.	RY	(12) C	30	0.06	2.32	0.011
60.	LP	(1) N	5	1272.	RY	(1) H	63	0.09	1.72	0.011
90.	BD	(1)Pt	1- N 2	190.	BD*	(1)Sb	14- O 19	0.19	0.50	0.009
90.	BD	(1)Pt	1- N 2	575.	RY	(1)Sb	14	0.07	1.84	0.010
90.	BD	(1)Pt	1- N 2	576.	RY	(2)Sb	14	0.07	2.02	0.010
90.	BD	(1)Pt	1- N 2	578.	RY	(4)Sb	14	0.22	1.37	0.016
90.	BD	(1)Pt	1- N 2	585.	RY	(11)Sb	14	0.31	1.66	0.020
90.	BD	(1)Pt	1- N 2	587.	RY	(13)Sb	14	1.35	1.99	0.046
90.	BD	(1)Pt	1- N 2	589.	RY	(15)Sb	14	0.31	1.64	0.020
90.	BD	(1)Pt	1- N 2	590.	RY	(16)Sb	14	0.14	2.21	0.016
90.	BD	(1)Pt	1- N 2	596.	RY	(22)Sb	14	0.05	2.33	0.010
90.	BD	(1)Pt	1- N 2	597.	RY	(23)Sb	14	0.09	2.23	0.013
90.	BD	(1)Pt	1- N 2	719.	RY	(4) O	19	0.06	1.84	0.009
90.	BD	(1)Pt	1- N 2	1010.	RY	(9) C	30	0.06	2.78	0.011

90.	BD	(1)Pt	1- N 2	1013.	RY	(12) C 30	0.07	2.21	0.011
90.	BD	(1)Pt	1- N 2	1085.	RY	(6) C 33	0.06	2.26	0.010
90.	BD	(1)Pt	1- N 2	1272.	RY	(1) H 63	0.11	1.62	0.012
91.	BD	(1)Pt	1- N 3	156.	LV	(1)Sb 14	0.12	0.47	0.007
91.	BD	(1)Pt	1- N 3	190.	BD*	(1)Sb 14- O 19	0.15	0.51	0.008
91.	BD	(1)Pt	1- N 3	575.	RY	(1)Sb 14	0.15	1.86	0.015
91.	BD	(1)Pt	1- N 3	578.	RY	(4)Sb 14	0.31	1.39	0.018
91.	BD	(1)Pt	1- N 3	585.	RY	(11)Sb 14	0.35	1.67	0.021
91.	BD	(1)Pt	1- N 3	587.	RY	(13)Sb 14	1.29	2.01	0.045
91.	BD	(1)Pt	1- N 3	589.	RY	(15)Sb 14	0.30	1.66	0.020
91.	BD	(1)Pt	1- N 3	590.	RY	(16)Sb 14	0.12	2.22	0.014
91.	BD	(1)Pt	1- N 3	596.	RY	(22)Sb 14	0.07	2.35	0.011
91.	BD	(1)Pt	1- N 3	597.	RY	(23)Sb 14	0.12	2.25	0.015
91.	BD	(1)Pt	1- N 3	691.	RY	(2) O 18	0.06	1.70	0.009
91.	BD	(1)Pt	1- N 3	719.	RY	(4) O 19	0.06	1.86	0.009
91.	BD	(1)Pt	1- N 3	1010.	RY	(9) C 30	0.07	2.80	0.012
91.	BD	(1)Pt	1- N 3	1013.	RY	(12) C 30	0.07	2.23	0.011
91.	BD	(1)Pt	1- N 3	1113.	RY	(8) C 34	0.06	2.61	0.011
91.	BD	(1)Pt	1- N 3	1272.	RY	(1) H 63	0.11	1.63	0.012
92.	BD	(1)Pt	1- N 4	587.	RY	(13)Sb 14	0.10	2.05	0.013
93.	BD	(1) N	2- C 6	587.	RY	(13)Sb 14	0.05	2.27	0.010
94.	BD	(1) N	2- H 35	587.	RY	(13)Sb 14	0.13	2.24	0.015
94.	BD	(1) N	2- H 35	589.	RY	(15)Sb 14	0.06	1.88	0.009
96.	BD	(1) N	3- H 36	585.	RY	(11)Sb 14	0.08	1.90	0.011
96.	BD	(1) N	3- H 36	587.	RY	(13)Sb 14	0.14	2.23	0.016
98.	BD	(1) N	4- C 11	585.	RY	(11)Sb 14	0.06	1.94	0.010
98.	BD	(1) N	4- C 11	587.	RY	(13)Sb 14	0.17	2.28	0.017
98.	BD	(1) N	4- C 11	589.	RY	(15)Sb 14	0.07	1.93	0.010
99.	BD	(1) N	5- C 10	587.	RY	(13)Sb 14	0.05	2.32	0.010
100.	BD	(1) N	5- C 12	587.	RY	(13)Sb 14	0.17	2.30	0.018
102.	BD	(1) C	6- H 37	587.	RY	(13)Sb 14	0.06	2.10	0.010
105.	BD	(1) C	7- H 39	587.	RY	(13)Sb 14	0.06	2.09	0.010
109.	BD	(1) C	9- C 10	587.	RY	(13)Sb 14	0.08	2.19	0.012
110.	BD	(1) C	9- H 43	587.	RY	(13)Sb 14	0.09	2.10	0.012
112.	BD	(1) C	10- H 45	587.	RY	(13)Sb 14	0.07	2.09	0.011
116.	BD	(1) C	11- H 49	587.	RY	(13)Sb 14	0.06	2.10	0.010
from unit 2 to unit 1									
29.	CR	(5)Sb 14		228.	RY	(7)Pt 1	0.05	4.52	0.014
32.	CR	(8)Sb 14		1152.	RY	(1) H 39	0.05	2.96	0.011
62.	LP	(1)Sb 14		157.	BD*	(1)Pt 1- N 2	0.54	0.40	0.013
62.	LP	(1)Sb 14		158.	BD*	(1)Pt 1- N 3	0.41	0.42	0.012
62.	LP	(1)Sb 14		159.	BD*	(1)Pt 1- N 4	0.13	0.13	0.004
62.	LP	(1)Sb 14		172.	BD*	(1) C 7- H 39	0.20	0.79	0.011
62.	LP	(1)Sb 14		232.	RY	(11)Pt 1	0.08	1.85	0.011
62.	LP	(1)Sb 14		235.	RY	(14)Pt 1	0.11	3.07	0.016
62.	LP	(1)Sb 14		236.	RY	(15)Pt 1	0.10	6.02	0.022
62.	LP	(1)Sb 14		237.	RY	(16)Pt 1	0.14	8.95	0.032
62.	LP	(1)Sb 14		243.	RY	(22)Pt 1	0.15	20.57	0.049
62.	LP	(1)Sb 14		244.	RY	(23)Pt 1	0.11	22.84	0.045
62.	LP	(1)Sb 14		245.	RY	(24)Pt 1	0.07	4.65	0.016
62.	LP	(1)Sb 14		250.	RY	(29)Pt 1	0.09	6.45	0.022
62.	LP	(1)Sb 14		252.	RY	(1) N 2	0.17	2.82	0.019
62.	LP	(1)Sb 14		253.	RY	(2) N 2	0.23	4.89	0.030
62.	LP	(1)Sb 14		254.	RY	(3) N 2	0.06	1.67	0.009
62.	LP	(1)Sb 14		256.	RY	(5) N 2	0.07	2.03	0.011
62.	LP	(1)Sb 14		264.	RY	(13) N 2	0.08	4.25	0.017
62.	LP	(1)Sb 14		278.	RY	(1) N 3	0.24	3.77	0.027
62.	LP	(1)Sb 14		279.	RY	(2) N 3	0.14	4.13	0.022
62.	LP	(1)Sb 14		281.	RY	(4) N 3	0.06	2.46	0.011
62.	LP	(1)Sb 14		283.	RY	(6) N 3	0.06	2.41	0.010
62.	LP	(1)Sb 14		304.	RY	(1) N 4	0.15	2.65	0.018
62.	LP	(1)Sb 14		305.	RY	(2) N 4	0.21	4.12	0.026
62.	LP	(1)Sb 14		330.	RY	(1) N 5	0.16	2.14	0.016
62.	LP	(1)Sb 14		331.	RY	(2) N 5	0.22	4.49	0.028
62.	LP	(1)Sb 14		343.	RY	(14) N 5	0.05	4.37	0.013
62.	LP	(1)Sb 14		1132.	RY	(1) H 35	0.05	1.78	0.009
62.	LP	(1)Sb 14		1137.	RY	(1) H 36	0.07	1.67	0.009
62.	LP	(1)Sb 14		1138.	RY	(2) H 36	0.05	2.52	0.010
62.	LP	(1)Sb 14		1152.	RY	(1) H 39	0.14	1.50	0.013
62.	LP	(1)Sb 14		1153.	RY	(2) H 39	0.05	2.88	0.011
70.	LP	(1) O 18		304.	RY	(1) N 4	0.10	3.04	0.016
70.	LP	(1) O 18		1182.	RY	(1) H 45	0.35	1.91	0.023
71.	LP	(2) O 18		304.	RY	(1) N 4	0.15	2.77	0.018
71.	LP	(2) O 18		306.	RY	(3) N 4	0.06	1.58	0.009
72.	LP	(3) O 18		304.	RY	(1) N 4	0.11	2.81	0.015
72.	LP	(3) O 18		1182.	RY	(1) H 45	0.19	1.67	0.016
86.	LP	(1) O 25		1217.	RY	(1) H 52	0.22	2.04	0.019
87.	LP	(2) O 25		1217.	RY	(1) H 52	0.68	1.78	0.031
123.	BD	(1)Sb 14- O 19		157.	BD*	(1)Pt 1- N 2	0.09	0.72	0.007
123.	BD	(1)Sb 14- O 19		158.	BD*	(1)Pt 1- N 3	0.08	0.74	0.007
123.	BD	(1)Sb 14- O 19		228.	RY	(7)Pt 1	0.06	3.37	0.012
123.	BD	(1)Sb 14- O 19		231.	RY	(10)Pt 1	0.08	2.39	0.012
123.	BD	(1)Sb 14- O 19		243.	RY	(22)Pt 1	0.06	20.89	0.032
123.	BD	(1)Sb 14- O 19		244.	RY	(23)Pt 1	0.05	23.16	0.031
123.	BD	(1)Sb 14- O 19		253.	RY	(2) N 2	0.07	5.21	0.017
123.	BD	(1)Sb 14- O 19		278.	RY	(1) N 3	0.08	4.09	0.016
123.	BD	(1)Sb 14- O 19		279.	RY	(2) N 3	0.06	4.45	0.014
123.	BD	(1)Sb 14- O 19		305.	RY	(2) N 4	0.07	4.44	0.016
123.	BD	(1)Sb 14- O 19		330.	RY	(1) N 5	0.06	2.46	0.011
123.	BD	(1)Sb 14- O 19		331.	RY	(2) N 5	0.07	4.81	0.016
124.	BD	(1)Sb 14- O 25		228.	RY	(7)Pt 1	0.05	3.39	0.012
129.	BD	(1) O 18- C 30		222.	RY	(1)Pt 1	0.14	3.14	0.019
129.	BD	(1) O 18- C 30		304.	RY	(1) N 4	0.25	3.25	0.025
129.	BD	(1) O 18- C 30		306.	RY	(3) N 4	0.06	2.06	0.010
129.	BD	(1) O 18- C 30		1182.	RY	(1) H 45	0.27	2.12	0.021
138.	BD	(1) O 25- C 33		1217.	RY	(1) H 52	0.13	2.23	0.015
within unit 2									
16.	CR	(1)Sb 13		573.	RY	(36)Sb 13	0.61	12.73	0.079
17.	CR	(2)Sb 13		187.	BD*	(1)Sb 13- O 16	0.92	4.74	0.059
17.	CR	(2)Sb 13		189.	BD*	(1)Sb 13- O 22	2.17	4.73	0.090
17.	CR	(2)Sb 13		541.	RY	(4)Sb 13	1.49	5.68	0.082

17. CR (2)Sb 13	543. RY (6)Sb 13	1.36	5.84	0.079
17. CR (2)Sb 13	551. RY (14)Sb 13	0.52	5.95	0.050
18. CR (3)Sb 13	188. BD* (1)Sb 13- O 21	2.53	4.74	0.098
18. CR (3)Sb 13	545. RY (8)Sb 13	0.60	5.94	0.053
18. CR (3)Sb 13	546. RY (9)Sb 13	0.87	6.02	0.064
18. CR (3)Sb 13	551. RY (14)Sb 13	0.58	5.95	0.052
19. CR (4)Sb 13	187. BD* (1)Sb 13- O 16	1.86	4.74	0.084
19. CR (4)Sb 13	189. BD* (1)Sb 13- O 22	1.23	4.73	0.068
19. CR (4)Sb 13	544. RY (7)Sb 13	0.76	5.90	0.060
19. CR (4)Sb 13	547. RY (10)Sb 13	0.51	5.81	0.049
20. CR (5)Sb 13	539. RY (2)Sb 13	1.14	3.20	0.054
20. CR (5)Sb 13	540. RY (3)Sb 13	0.99	3.23	0.051
20. CR (5)Sb 13	541. RY (4)Sb 13	2.90	2.88	0.082
20. CR (5)Sb 13	542. RY (5)Sb 13	6.15	3.00	0.121
20. CR (5)Sb 13	546. RY (9)Sb 13	0.74	3.22	0.044
20. CR (5)Sb 13	548. RY (11)Sb 13	1.76	2.90	0.064
20. CR (5)Sb 13	551. RY (14)Sb 13	1.69	3.15	0.065
20. CR (5)Sb 13	552. RY (15)Sb 13	0.76	3.85	0.048
20. CR (5)Sb 13	554. RY (17)Sb 13	1.37	3.16	0.059
20. CR (5)Sb 13	556. RY (19)Sb 13	2.27	3.34	0.078
20. CR (5)Sb 13	561. RY (24)Sb 13	1.08	3.91	0.058
20. CR (5)Sb 13	769. RY (2) O 21	0.98	2.99	0.048
21. CR (6)Sb 13	538. RY (1)Sb 13	4.81	3.16	0.110
21. CR (6)Sb 13	539. RY (2)Sb 13	2.19	3.20	0.075
21. CR (6)Sb 13	540. RY (3)Sb 13	3.44	3.24	0.094
21. CR (6)Sb 13	545. RY (8)Sb 13	0.89	3.15	0.047
21. CR (6)Sb 13	551. RY (14)Sb 13	2.50	3.16	0.079
21. CR (6)Sb 13	553. RY (16)Sb 13	0.93	3.08	0.048
21. CR (6)Sb 13	563. RY (26)Sb 13	0.71	4.37	0.050
21. CR (6)Sb 13	564. RY (27)Sb 13	0.55	4.67	0.045
21. CR (6)Sb 13	613. RY (2) O 15	1.73	3.06	0.065
21. CR (6)Sb 13	638. RY (1) O 16	1.02	3.07	0.050
21. CR (6)Sb 13	639. RY (2) O 16	1.22	2.94	0.053
21. CR (6)Sb 13	640. RY (3) O 16	0.59	3.14	0.038
21. CR (6)Sb 13	795. RY (2) O 22	0.90	3.04	0.047
22. CR (7)Sb 13	539. RY (2)Sb 13	7.13	3.20	0.135
22. CR (7)Sb 13	540. RY (3)Sb 13	0.56	3.23	0.038
22. CR (7)Sb 13	546. RY (9)Sb 13	2.07	3.22	0.073
22. CR (7)Sb 13	549. RY (12)Sb 13	0.63	3.11	0.039
22. CR (7)Sb 13	552. RY (15)Sb 13	1.02	3.84	0.056
22. CR (7)Sb 13	553. RY (16)Sb 13	2.59	3.07	0.080
22. CR (7)Sb 13	554. RY (17)Sb 13	1.27	3.16	0.057
22. CR (7)Sb 13	557. RY (20)Sb 13	2.55	3.48	0.084
22. CR (7)Sb 13	558. RY (21)Sb 13	0.63	3.91	0.044
22. CR (7)Sb 13	560. RY (23)Sb 13	1.26	3.91	0.063
23. CR (8)Sb 13	538. RY (1)Sb 13	1.54	3.16	0.062
23. CR (8)Sb 13	541. RY (4)Sb 13	1.69	2.88	0.062
23. CR (8)Sb 13	542. RY (5)Sb 13	2.23	3.00	0.073
23. CR (8)Sb 13	543. RY (6)Sb 13	1.11	3.04	0.052
23. CR (8)Sb 13	544. RY (7)Sb 13	1.10	3.11	0.052
23. CR (8)Sb 13	546. RY (9)Sb 13	1.76	3.22	0.067
23. CR (8)Sb 13	550. RY (13)Sb 13	3.05	3.08	0.087
23. CR (8)Sb 13	551. RY (14)Sb 13	0.54	3.15	0.037
23. CR (8)Sb 13	552. RY (15)Sb 13	0.79	3.85	0.049
23. CR (8)Sb 13	555. RY (18)Sb 13	0.57	3.81	0.041
23. CR (8)Sb 13	557. RY (20)Sb 13	0.57	3.49	0.040
23. CR (8)Sb 13	561. RY (24)Sb 13	0.78	3.91	0.049
23. CR (8)Sb 13	564. RY (27)Sb 13	1.46	4.67	0.074
23. CR (8)Sb 13	565. RY (28)Sb 13	0.80	5.51	0.059
23. CR (8)Sb 13	639. RY (2) O 16	0.51	2.94	0.034
23. CR (8)Sb 13	768. RY (1) O 21	1.10	3.09	0.052
23. CR (8)Sb 13	769. RY (2) O 21	0.58	2.99	0.037
23. CR (8)Sb 13	795. RY (2) O 22	0.58	3.04	0.037
24. CR (9)Sb 13	538. RY (1)Sb 13	2.77	3.16	0.083
24. CR (9)Sb 13	540. RY (3)Sb 13	1.40	3.23	0.060
24. CR (9)Sb 13	542. RY (5)Sb 13	1.83	3.00	0.066
24. CR (9)Sb 13	546. RY (9)Sb 13	1.85	3.22	0.069
24. CR (9)Sb 13	547. RY (10)Sb 13	1.53	3.01	0.061
24. CR (9)Sb 13	550. RY (13)Sb 13	1.47	3.08	0.060
24. CR (9)Sb 13	551. RY (14)Sb 13	0.57	3.15	0.038
24. CR (9)Sb 13	553. RY (16)Sb 13	1.09	3.08	0.052
24. CR (9)Sb 13	554. RY (17)Sb 13	1.07	3.16	0.052
24. CR (9)Sb 13	556. RY (19)Sb 13	2.07	3.34	0.074
24. CR (9)Sb 13	560. RY (23)Sb 13	0.69	3.91	0.046
24. CR (9)Sb 13	561. RY (24)Sb 13	0.87	3.91	0.052
24. CR (9)Sb 13	562. RY (25)Sb 13	0.84	4.14	0.053
24. CR (9)Sb 13	564. RY (27)Sb 13	1.09	4.67	0.064
24. CR (9)Sb 13	640. RY (3) O 16	0.64	3.14	0.040
25. CR (1)Sb 14	611. RY (37)Sb 14	0.65	22.14	0.107
26. CR (2)Sb 14	156. LV (1)Sb 14	2.92	4.70	0.105
26. CR (2)Sb 14	190. BD* (1)Sb 14- O 19	0.89	4.74	0.058
26. CR (2)Sb 14	578. RY (4)Sb 14	2.06	5.62	0.096
27. CR (3)Sb 14	156. LV (1)Sb 14	1.03	4.69	0.062
27. CR (3)Sb 14	190. BD* (1)Sb 14- O 19	1.76	4.74	0.081
27. CR (3)Sb 14	576. RY (2)Sb 14	0.52	6.26	0.051
27. CR (3)Sb 14	582. RY (8)Sb 14	1.06	5.81	0.070
27. CR (3)Sb 14	589. RY (15)Sb 14	0.78	5.89	0.061
28. CR (4)Sb 14	191. BD* (1)Sb 14- O 25	2.58	4.75	0.099
28. CR (4)Sb 14	577. RY (3)Sb 14	0.74	6.13	0.060
28. CR (4)Sb 14	584. RY (10)Sb 14	0.99	5.98	0.069
28. CR (4)Sb 14	595. RY (21)Sb 14	0.53	6.28	0.051
29. CR (5)Sb 14	576. RY (2)Sb 14	3.15	3.47	0.093
29. CR (5)Sb 14	577. RY (3)Sb 14	1.71	3.34	0.067
29. CR (5)Sb 14	578. RY (4)Sb 14	2.28	2.82	0.072
29. CR (5)Sb 14	579. RY (5)Sb 14	0.68	3.18	0.041
29. CR (5)Sb 14	580. RY (6)Sb 14	1.10	3.15	0.053
29. CR (5)Sb 14	581. RY (7)Sb 14	0.89	3.18	0.048
29. CR (5)Sb 14	586. RY (12)Sb 14	1.04	3.47	0.054
29. CR (5)Sb 14	587. RY (13)Sb 14	1.27	3.44	0.059
29. CR (5)Sb 14	589. RY (15)Sb 14	2.25	3.09	0.074
29. CR (5)Sb 14	590. RY (16)Sb 14	0.65	3.66	0.043
29. CR (5)Sb 14	591. RY (17)Sb 14	0.69	3.68	0.045
29. CR (5)Sb 14	594. RY (20)Sb 14	0.71	4.23	0.049

29. CR (5)Sb 14	596. RY (22)Sb 14	0.54	3.78	0.040
29. CR (5)Sb 14	597. RY (23)Sb 14	1.25	3.68	0.061
29. CR (5)Sb 14	691. RY (2) O 18	1.74	3.13	0.066
29. CR (5)Sb 14	716. RY (1) O 19	1.25	3.12	0.056
29. CR (5)Sb 14	717. RY (2) O 19	1.29	3.07	0.056
29. CR (5)Sb 14	718. RY (3) O 19	0.65	3.22	0.041
30. CR (6)Sb 14	575. RY (1)Sb 14	1.95	3.29	0.071
30. CR (6)Sb 14	576. RY (2)Sb 14	2.27	3.47	0.079
30. CR (6)Sb 14	578. RY (4)Sb 14	1.03	2.82	0.048
30. CR (6)Sb 14	579. RY (5)Sb 14	4.01	3.17	0.101
30. CR (6)Sb 14	580. RY (6)Sb 14	3.12	3.15	0.088
30. CR (6)Sb 14	584. RY (10)Sb 14	2.03	3.18	0.072
30. CR (6)Sb 14	591. RY (17)Sb 14	1.00	3.68	0.054
30. CR (6)Sb 14	594. RY (20)Sb 14	2.15	4.23	0.085
30. CR (6)Sb 14	598. RY (24)Sb 14	0.76	3.79	0.048
30. CR (6)Sb 14	601. RY (27)Sb 14	0.53	4.72	0.045
30. CR (6)Sb 14	847. RY (2) O 24	1.15	3.06	0.053
30. CR (6)Sb 14	873. RY (2) O 25	1.01	3.03	0.049
31. CR (7)Sb 14	575. RY (1)Sb 14	4.78	3.28	0.112
31. CR (7)Sb 14	577. RY (3)Sb 14	1.88	3.34	0.071
31. CR (7)Sb 14	580. RY (6)Sb 14	0.53	3.14	0.036
31. CR (7)Sb 14	583. RY (9)Sb 14	0.56	3.26	0.038
31. CR (7)Sb 14	585. RY (11)Sb 14	0.57	3.10	0.037
31. CR (7)Sb 14	590. RY (16)Sb 14	2.81	3.65	0.090
31. CR (7)Sb 14	591. RY (17)Sb 14	1.47	3.67	0.066
31. CR (7)Sb 14	592. RY (18)Sb 14	0.72	3.16	0.043
31. CR (7)Sb 14	596. RY (22)Sb 14	5.30	3.78	0.126
31. CR (7)Sb 14	872. RY (1) O 25	1.33	3.17	0.058
32. CR (8)Sb 14	576. RY (2)Sb 14	2.25	3.47	0.079
32. CR (8)Sb 14	578. RY (4)Sb 14	1.24	2.82	0.053
32. CR (8)Sb 14	579. RY (5)Sb 14	4.38	3.17	0.105
32. CR (8)Sb 14	582. RY (8)Sb 14	1.11	3.02	0.052
32. CR (8)Sb 14	583. RY (9)Sb 14	2.62	3.26	0.083
32. CR (8)Sb 14	586. RY (12)Sb 14	0.86	3.47	0.049
32. CR (8)Sb 14	589. RY (15)Sb 14	3.00	3.09	0.086
32. CR (8)Sb 14	592. RY (18)Sb 14	0.53	3.16	0.036
32. CR (8)Sb 14	594. RY (20)Sb 14	1.08	4.23	0.060
32. CR (8)Sb 14	595. RY (21)Sb 14	2.28	3.48	0.080
32. CR (8)Sb 14	719. RY (4) O 19	0.69	3.29	0.043
32. CR (8)Sb 14	847. RY (2) O 24	0.61	3.05	0.039
33. CR (9)Sb 14	575. RY (1)Sb 14	2.31	3.29	0.078
33. CR (9)Sb 14	577. RY (3)Sb 14	2.16	3.34	0.076
33. CR (9)Sb 14	583. RY (9)Sb 14	0.52	3.26	0.037
33. CR (9)Sb 14	584. RY (10)Sb 14	1.92	3.18	0.070
33. CR (9)Sb 14	585. RY (11)Sb 14	1.03	3.11	0.051
33. CR (9)Sb 14	586. RY (12)Sb 14	1.98	3.47	0.074
33. CR (9)Sb 14	592. RY (18)Sb 14	1.39	3.16	0.059
33. CR (9)Sb 14	593. RY (19)Sb 14	2.83	3.73	0.092
33. CR (9)Sb 14	595. RY (21)Sb 14	1.02	3.49	0.053
33. CR (9)Sb 14	597. RY (23)Sb 14	1.65	3.68	0.070
33. CR (9)Sb 14	598. RY (24)Sb 14	0.86	3.79	0.051
33. CR (9)Sb 14	873. RY (2) O 25	0.92	3.03	0.047
33. CR (9)Sb 14	874. RY (3) O 25	1.45	3.33	0.062
34. CR (1) O 15	192. BD* (1) O 15- C 27	0.98	21.40	0.129
34. CR (1) O 15	628. RY (17) O 15	14.92	43.29	0.717
34. CR (1) O 15	629. RY (18) O 15	4.26	30.70	0.323
34. CR (1) O 15	630. RY (19) O 15	5.26	30.13	0.355
34. CR (1) O 15	631. RY (20) O 15	1.91	28.71	0.209
34. CR (1) O 15	632. RY (21) O 15	2.43	28.02	0.233
34. CR (1) O 15	633. RY (22) O 15	2.45	28.74	0.237
34. CR (1) O 15	634. RY (23) O 15	2.39	28.72	0.234
34. CR (1) O 15	636. RY (25) O 15	1.00	27.35	0.148
34. CR (1) O 15	637. RY (26) O 15	0.51	26.79	0.104
35. CR (1) O 16	193. BD* (1) O 16- C 28	0.75	21.22	0.112
35. CR (1) O 16	651. RY (14) O 16	0.57	26.12	0.109
35. CR (1) O 16	653. RY (16) O 16	19.24	56.38	0.930
35. CR (1) O 16	654. RY (17) O 16	2.55	28.34	0.240
35. CR (1) O 16	655. RY (18) O 16	1.90	28.00	0.206
35. CR (1) O 16	660. RY (23) O 16	0.60	26.52	0.113
36. CR (1) O 17	194. BD* (1) O 17- C 27	1.05	21.46	0.134
36. CR (1) O 17	195. BD* (1) O 17- H 53	0.55	21.46	0.097
36. CR (1) O 17	676. RY (13) O 17	2.30	29.12	0.231
36. CR (1) O 17	677. RY (14) O 17	3.34	30.27	0.284
36. CR (1) O 17	678. RY (15) O 17	0.64	27.66	0.118
36. CR (1) O 17	679. RY (16) O 17	0.50	27.49	0.105
36. CR (1) O 17	680. RY (17) O 17	0.97	25.23	0.139
36. CR (1) O 17	681. RY (18) O 17	3.21	29.01	0.273
36. CR (1) O 17	683. RY (20) O 17	9.24	35.74	0.513
36. CR (1) O 17	684. RY (21) O 17	6.51	32.44	0.410
36. CR (1) O 17	685. RY (22) O 17	1.16	27.13	0.159
36. CR (1) O 17	686. RY (23) O 17	0.76	27.45	0.129
36. CR (1) O 17	688. RY (25) O 17	6.41	30.51	0.395
36. CR (1) O 17	689. RY (26) O 17	3.88	29.98	0.305
36. CR (1) O 17	929. RY (6) C 27	0.55	24.17	0.103
37. CR (1) O 18	196. BD* (1) O 18- C 30	0.82	21.34	0.118
37. CR (1) O 18	691. RY (2) O 18	0.53	22.40	0.097
37. CR (1) O 18	702. RY (13) O 18	0.88	25.17	0.133
37. CR (1) O 18	704. RY (15) O 18	17.74	50.62	0.846
37. CR (1) O 18	706. RY (17) O 18	5.18	31.22	0.359
37. CR (1) O 18	707. RY (18) O 18	1.40	27.35	0.174
37. CR (1) O 18	709. RY (20) O 18	2.24	28.08	0.224
37. CR (1) O 18	714. RY (25) O 18	0.52	26.91	0.106
37. CR (1) O 18	715. RY (26) O 18	0.54	25.63	0.105
38. CR (1) O 19	197. BD* (1) O 19- C 29	0.82	21.26	0.118
38. CR (1) O 19	730. RY (15) O 19	1.79	27.75	0.199
38. CR (1) O 19	731. RY (16) O 19	19.58	55.50	0.930
38. CR (1) O 19	732. RY (17) O 19	1.19	27.64	0.162
38. CR (1) O 19	733. RY (18) O 19	0.73	27.06	0.125
38. CR (1) O 19	735. RY (20) O 19	0.79	27.25	0.131
39. CR (1) O 20	198. BD* (1) O 20- C 30	1.07	21.51	0.136
39. CR (1) O 20	199. BD* (1) O 20- H 54	0.53	21.46	0.095
39. CR (1) O 20	755. RY (14) O 20	1.37	28.43	0.176
39. CR (1) O 20	756. RY (15) O 20	1.99	29.62	0.217

39.	CR	(1)	O	20	758.	RY	(17)	O	20	0.70	27.36	0.124
39.	CR	(1)	O	20	759.	RY	(18)	O	20	6.00	31.56	0.388
39.	CR	(1)	O	20	761.	RY	(20)	O	20	7.78	33.01	0.452
39.	CR	(1)	O	20	762.	RY	(21)	O	20	6.70	32.31	0.415
39.	CR	(1)	O	20	764.	RY	(23)	O	20	1.07	27.53	0.153
39.	CR	(1)	O	20	765.	RY	(24)	O	20	2.03	28.30	0.214
39.	CR	(1)	O	20	766.	RY	(25)	O	20	8.57	34.43	0.485
39.	CR	(1)	O	20	767.	RY	(26)	O	20	1.94	28.02	0.208
40.	CR	(1)	O	21	200.	BD*	(1)	O	21- C 32	0.73	21.21	0.111
40.	CR	(1)	O	21	783.	RY	(16)	O	21	18.52	52.68	0.882
40.	CR	(1)	O	21	784.	RY	(17)	O	21	1.72	28.18	0.197
40.	CR	(1)	O	21	785.	RY	(18)	O	21	2.81	28.73	0.254
40.	CR	(1)	O	21	786.	RY	(19)	O	21	0.89	27.12	0.139
40.	CR	(1)	O	21	788.	RY	(21)	O	21	0.90	26.89	0.139
40.	CR	(1)	O	21	793.	RY	(26)	O	21	2.99	28.68	0.262
41.	CR	(1)	O	22	201.	BD*	(1)	O	22- C 31	0.96	21.36	0.128
41.	CR	(1)	O	22	805.	RY	(12)	O	22	0.54	24.91	0.104
41.	CR	(1)	O	22	807.	RY	(14)	O	22	0.52	27.19	0.106
41.	CR	(1)	O	22	809.	RY	(16)	O	22	1.30	27.37	0.168
41.	CR	(1)	O	22	810.	RY	(17)	O	22	16.03	45.06	0.759
41.	CR	(1)	O	22	811.	RY	(18)	O	22	10.32	36.59	0.549
41.	CR	(1)	O	22	814.	RY	(21)	O	22	1.41	27.31	0.175
41.	CR	(1)	O	22	815.	RY	(22)	O	22	0.68	27.48	0.122
41.	CR	(1)	O	22	817.	RY	(24)	O	22	0.84	27.24	0.135
41.	CR	(1)	O	22	819.	RY	(26)	O	22	0.50	25.78	0.102
42.	CR	(1)	O	23	202.	BD*	(1)	O	23- C 31	1.06	21.51	0.135
42.	CR	(1)	O	23	203.	BD*	(1)	O	23- H 55	0.53	21.46	0.095
42.	CR	(1)	O	23	832.	RY	(13)	O	23	1.25	29.34	0.171
42.	CR	(1)	O	23	834.	RY	(15)	O	23	1.12	25.78	0.151
42.	CR	(1)	O	23	838.	RY	(19)	O	23	13.26	40.20	0.652
42.	CR	(1)	O	23	839.	RY	(20)	O	23	2.58	28.65	0.243
42.	CR	(1)	O	23	840.	RY	(21)	O	23	2.95	29.06	0.262
42.	CR	(1)	O	23	841.	RY	(22)	O	23	0.87	27.32	0.138
42.	CR	(1)	O	23	842.	RY	(23)	O	23	0.86	27.43	0.137
42.	CR	(1)	O	23	843.	RY	(24)	O	23	9.47	34.93	0.513
42.	CR	(1)	O	23	845.	RY	(26)	O	23	2.38	29.44	0.236
43.	CR	(1)	O	24	204.	BD*	(1)	O	24- C 34	0.93	21.37	0.126
43.	CR	(1)	O	24	862.	RY	(17)	O	24	18.53	53.20	0.886
43.	CR	(1)	O	24	864.	RY	(19)	O	24	1.96	27.62	0.208
43.	CR	(1)	O	24	865.	RY	(20)	O	24	0.53	27.19	0.107
43.	CR	(1)	O	24	868.	RY	(23)	O	24	5.04	30.50	0.350
44.	CR	(1)	O	25	205.	BD*	(1)	O	25- C 33	0.78	21.24	0.115
44.	CR	(1)	O	25	887.	RY	(16)	O	25	2.89	29.10	0.259
44.	CR	(1)	O	25	889.	RY	(18)	O	25	0.58	26.86	0.112
44.	CR	(1)	O	25	894.	RY	(23)	O	25	1.11	27.20	0.155
44.	CR	(1)	O	25	897.	RY	(26)	O	25	19.62	56.11	0.937
45.	CR	(1)	O	26	206.	BD*	(1)	O	26- C 34	1.08	21.48	0.136
45.	CR	(1)	O	26	207.	BD*	(1)	O	26- H 56	0.53	21.46	0.095
45.	CR	(1)	O	26	911.	RY	(14)	O	26	3.74	30.18	0.300
45.	CR	(1)	O	26	912.	RY	(15)	O	26	2.04	29.76	0.220
45.	CR	(1)	O	26	913.	RY	(16)	O	26	0.69	27.77	0.124
45.	CR	(1)	O	26	914.	RY	(17)	O	26	1.25	27.91	0.166
45.	CR	(1)	O	26	915.	RY	(18)	O	26	4.89	30.32	0.344
45.	CR	(1)	O	26	917.	RY	(20)	O	26	1.55	28.29	0.187
45.	CR	(1)	O	26	918.	RY	(21)	O	26	11.09	36.40	0.567
45.	CR	(1)	O	26	919.	RY	(22)	O	26	3.71	30.46	0.300
45.	CR	(1)	O	26	920.	RY	(23)	O	26	1.51	27.91	0.183
45.	CR	(1)	O	26	921.	RY	(24)	O	26	2.62	28.23	0.243
45.	CR	(1)	O	26	922.	RY	(25)	O	26	5.12	30.38	0.352
45.	CR	(1)	O	26	923.	RY	(26)	O	26	0.56	27.28	0.110
45.	CR	(1)	O	26	1111.	RY	(6)	C	34	0.56	24.17	0.104
46.	CR	(1)	C	27	192.	BD*	(1)	O	15- C 27	1.21	11.92	0.107
46.	CR	(1)	C	27	194.	BD*	(1)	O	17- C 27	1.07	11.93	0.101
46.	CR	(1)	C	27	208.	BD*	(1)	C	27- C 28	1.06	11.85	0.100
46.	CR	(1)	C	27	924.	RY	(1)	C	27	0.76	12.84	0.088
46.	CR	(1)	C	27	928.	RY	(5)	C	27	0.90	13.83	0.100
46.	CR	(1)	C	27	933.	RY	(10)	C	27	0.58	13.97	0.081
46.	CR	(1)	C	27	936.	RY	(13)	C	27	0.50	14.42	0.076
46.	CR	(1)	C	27	939.	RY	(16)	C	27	1.00	14.97	0.109
46.	CR	(1)	C	27	941.	RY	(18)	C	27	0.59	14.52	0.082
46.	CR	(1)	C	27	942.	RY	(19)	C	27	3.72	17.17	0.226
46.	CR	(1)	C	27	943.	RY	(20)	C	27	13.49	23.45	0.502
46.	CR	(1)	C	27	944.	RY	(21)	C	27	9.04	19.43	0.374
46.	CR	(1)	C	27	947.	RY	(24)	C	27	1.91	15.51	0.154
46.	CR	(1)	C	27	948.	RY	(25)	C	27	0.56	15.37	0.083
46.	CR	(1)	C	27	965.	RY	(16)	C	28	0.53	15.51	0.081
46.	CR	(1)	C	27	1242.	RY	(1)	H	57	0.51	12.73	0.072
47.	CR	(1)	C	28	193.	BD*	(1)	O	16- C 28	1.10	11.69	0.101
47.	CR	(1)	C	28	208.	BD*	(1)	C	27- C 28	0.93	11.83	0.094
47.	CR	(1)	C	28	210.	BD*	(1)	C	28- C 29	1.10	11.84	0.102
47.	CR	(1)	C	28	211.	BD*	(1)	C	28- H 58	0.72	11.96	0.083
47.	CR	(1)	C	28	936.	RY	(13)	C	27	0.75	14.40	0.093
47.	CR	(1)	C	28	953.	RY	(4)	C	28	1.02	13.07	0.103
47.	CR	(1)	C	28	956.	RY	(7)	C	28	0.89	13.50	0.098
47.	CR	(1)	C	28	961.	RY	(12)	C	28	1.44	15.52	0.133
47.	CR	(1)	C	28	962.	RY	(13)	C	28	1.09	15.05	0.114
47.	CR	(1)	C	28	963.	RY	(14)	C	28	2.26	15.57	0.167
47.	CR	(1)	C	28	967.	RY	(18)	C	28	0.93	14.97	0.105
47.	CR	(1)	C	28	969.	RY	(20)	C	28	1.93	16.10	0.157
47.	CR	(1)	C	28	971.	RY	(22)	C	28	7.19	18.19	0.323
47.	CR	(1)	C	28	972.	RY	(23)	C	28	11.23	20.20	0.425
47.	CR	(1)	C	28	973.	RY	(24)	C	28	4.49	16.88	0.246
47.	CR	(1)	C	28	975.	RY	(26)	C	28	0.75	15.46	0.096
47.	CR	(1)	C	28	985.	RY	(10)	C	29	0.54	15.26	0.081
48.	CR	(1)	C	29	197.	BD*	(1)	O	19- C 29	1.15	11.74	0.104
48.	CR	(1)	C	29	210.	BD*	(1)	C	28- C 29	1.13	11.83	0.103
48.	CR	(1)	C	29	212.	BD*	(1)	C	29- C 30	0.86	11.81	0.090
48.	CR	(1)	C	29	213.	BD*	(1)	C	29- H 59	0.69	11.95	0.081
48.	CR	(1)	C	29	965.	RY	(16)	C	28	0.53	15.49	0.081
48.	CR	(1)	C	29	978.	RY	(3)	C	29	0.68	13.04	0.084
48.	CR	(1)	C	29	979.	RY	(4)	C	29	0.59	13.13	0.079
48.	CR	(1)	C	29	985.	RY	(10)	C	29	1.91	15.25	0.152
48.	CR	(1)	C	29	989.	RY	(14)	C	29	1.13	15.34	0.118

48. CR (1) C 29	995. RY (20) C 29	2.97	16.48	0.197
48. CR (1) C 29	996. RY (21) C 29	2.82	16.71	0.194
48. CR (1) C 29	997. RY (22) C 29	13.46	20.75	0.472
48. CR (1) C 29	998. RY (23) C 29	4.21	16.36	0.234
48. CR (1) C 29	999. RY (24) C 29	1.68	15.80	0.146
48. CR (1) C 29	1000. RY (25) C 29	3.32	16.72	0.210
48. CR (1) C 29	1017. RY (16) C 30	0.98	14.32	0.106
49. CR (1) C 30	196. BD* (1) O 18- C 30	1.20	11.84	0.106
49. CR (1) C 30	198. BD* (1) O 20- C 30	0.96	11.95	0.096
49. CR (1) C 30	212. BD* (1) C 29- C 30	1.08	11.83	0.101
49. CR (1) C 30	1002. RY (1) C 30	0.55	12.89	0.075
49. CR (1) C 30	1019. RY (18) C 30	1.99	14.90	0.154
49. CR (1) C 30	1020. RY (19) C 30	1.15	15.69	0.120
49. CR (1) C 30	1022. RY (21) C 30	1.43	15.74	0.134
49. CR (1) C 30	1023. RY (22) C 30	3.67	16.91	0.222
49. CR (1) C 30	1024. RY (23) C 30	11.55	21.06	0.440
49. CR (1) C 30	1025. RY (24) C 30	11.93	22.21	0.459
49. CR (1) C 30	1026. RY (25) C 30	1.60	15.91	0.142
49. CR (1) C 30	1027. RY (26) C 30	0.69	15.27	0.092
50. CR (1) C 31	201. BD* (1) O 22- C 31	1.16	11.87	0.105
50. CR (1) C 31	202. BD* (1) O 23- C 31	0.97	11.95	0.096
50. CR (1) C 31	215. BD* (1) C 31- C 32	1.02	11.86	0.098
50. CR (1) C 31	1028. RY (1) C 31	0.58	12.88	0.077
50. CR (1) C 31	1045. RY (18) C 31	0.62	14.36	0.084
50. CR (1) C 31	1046. RY (19) C 31	1.02	15.68	0.113
50. CR (1) C 31	1047. RY (20) C 31	1.80	15.80	0.151
50. CR (1) C 31	1048. RY (21) C 31	1.86	16.00	0.154
50. CR (1) C 31	1049. RY (22) C 31	5.28	16.73	0.265
50. CR (1) C 31	1050. RY (23) C 31	1.02	15.40	0.112
50. CR (1) C 31	1051. RY (24) C 31	17.06	27.79	0.615
50. CR (1) C 31	1053. RY (26) C 31	0.61	15.22	0.086
51. CR (1) C 32	200. BD* (1) O 21- C 32	1.10	11.69	0.101
51. CR (1) C 32	215. BD* (1) C 31- C 32	0.89	11.84	0.091
51. CR (1) C 32	217. BD* (1) C 32- C 33	1.13	11.82	0.103
51. CR (1) C 32	218. BD* (1) C 32- H 62	0.71	11.95	0.083
51. CR (1) C 32	1043. RY (16) C 31	1.20	13.90	0.115
51. CR (1) C 32	1056. RY (3) C 32	0.66	13.03	0.083
51. CR (1) C 32	1063. RY (10) C 32	1.73	15.06	0.144
51. CR (1) C 32	1067. RY (14) C 32	1.45	15.71	0.135
51. CR (1) C 32	1073. RY (20) C 32	1.64	15.93	0.144
51. CR (1) C 32	1074. RY (21) C 32	2.05	15.53	0.159
51. CR (1) C 32	1075. RY (22) C 32	2.63	16.42	0.186
51. CR (1) C 32	1076. RY (23) C 32	17.20	24.40	0.578
51. CR (1) C 32	1077. RY (24) C 32	0.97	15.58	0.110
51. CR (1) C 32	1095. RY (16) C 33	0.70	16.76	0.096
52. CR (1) C 33	205. BD* (1) O 25- C 33	1.14	11.72	0.103
52. CR (1) C 33	217. BD* (1) C 32- C 33	1.08	11.82	0.101
52. CR (1) C 33	219. BD* (1) C 33- C 34	0.94	11.83	0.094
52. CR (1) C 33	220. BD* (1) C 33- H 63	0.71	11.96	0.082
52. CR (1) C 33	1063. RY (10) C 32	0.64	15.06	0.087
52. CR (1) C 33	1083. RY (4) C 33	1.15	13.10	0.110
52. CR (1) C 33	1086. RY (7) C 33	1.41	13.65	0.124
52. CR (1) C 33	1091. RY (12) C 33	1.50	15.59	0.137
52. CR (1) C 33	1092. RY (13) C 33	0.55	14.96	0.081
52. CR (1) C 33	1093. RY (14) C 33	2.44	15.58	0.174
52. CR (1) C 33	1095. RY (16) C 33	2.04	16.76	0.165
52. CR (1) C 33	1097. RY (18) C 33	0.66	15.34	0.090
52. CR (1) C 33	1099. RY (20) C 33	3.54	16.74	0.217
52. CR (1) C 33	1101. RY (22) C 33	4.70	16.47	0.248
52. CR (1) C 33	1102. RY (23) C 33	6.66	18.14	0.310
52. CR (1) C 33	1103. RY (24) C 33	7.88	18.25	0.339
52. CR (1) C 33	1104. RY (25) C 33	0.95	15.56	0.109
52. CR (1) C 33	1105. RY (26) C 33	1.68	15.72	0.145
52. CR (1) C 33	1120. RY (15) C 34	0.67	13.74	0.085
53. CR (1) C 34	204. BD* (1) O 24- C 34	1.23	11.90	0.108
53. CR (1) C 34	206. BD* (1) O 26- C 34	1.04	11.94	0.100
53. CR (1) C 34	219. BD* (1) C 33- C 34	1.07	11.85	0.100
53. CR (1) C 34	1106. RY (1) C 34	0.65	12.86	0.082
53. CR (1) C 34	1110. RY (5) C 34	1.14	13.82	0.112
53. CR (1) C 34	1118. RY (13) C 34	0.61	14.21	0.083
53. CR (1) C 34	1124. RY (19) C 34	11.65	21.97	0.452
53. CR (1) C 34	1125. RY (20) C 34	1.03	15.50	0.113
53. CR (1) C 34	1126. RY (21) C 34	11.98	21.59	0.454
53. CR (1) C 34	1128. RY (23) C 34	0.69	15.34	0.092
53. CR (1) C 34	1129. RY (24) C 34	4.76	16.66	0.251
53. CR (1) C 34	1131. RY (26) C 34	0.59	15.24	0.085
53. CR (1) C 34	1277. RY (1) H 64	0.50	12.74	0.072
61. LP (1) Sb 13	187. BD* (1) Sb 13- O 16	12.00	0.48	0.068
61. LP (1) Sb 13	188. BD* (1) Sb 13- O 21	11.33	0.48	0.066
61. LP (1) Sb 13	192. BD* (1) O 15- C 27	0.57	0.69	0.018
61. LP (1) Sb 13	193. BD* (1) O 16- C 28	0.64	0.48	0.016
61. LP (1) Sb 13	200. BD* (1) O 21- C 32	0.61	0.48	0.015
61. LP (1) Sb 13	538. RY (1) Sb 13	1.38	1.69	0.043
61. LP (1) Sb 13	539. RY (2) Sb 13	0.62	1.73	0.029
61. LP (1) Sb 13	548. RY (11) Sb 13	1.14	1.43	0.036
61. LP (1) Sb 13	549. RY (12) Sb 13	1.03	1.65	0.037
61. LP (1) Sb 13	550. RY (13) Sb 13	0.54	1.61	0.026
61. LP (1) Sb 13	551. RY (14) Sb 13	2.16	1.69	0.054
61. LP (1) Sb 13	553. RY (16) Sb 13	0.57	1.61	0.027
61. LP (1) Sb 13	555. RY (18) Sb 13	0.82	2.34	0.039
61. LP (1) Sb 13	573. RY (36) Sb 13	0.79	6.63	0.064
61. LP (1) Sb 13	613. RY (2) O 15	0.71	1.59	0.030
61. LP (1) Sb 13	638. RY (1) O 16	0.59	1.59	0.027
61. LP (1) Sb 13	768. RY (1) O 21	0.53	1.63	0.026
61. LP (1) Sb 13	769. RY (2) O 21	0.60	1.52	0.027
61. LP (1) Sb 13	795. RY (2) O 22	0.56	1.57	0.026
62. LP (1) Sb 14	190. BD* (1) Sb 14- O 19	11.19	0.48	0.065
62. LP (1) Sb 14	191. BD* (1) Sb 14- O 25	11.66	0.49	0.068
62. LP (1) Sb 14	196. BD* (1) O 18- C 30	0.55	0.61	0.016
62. LP (1) Sb 14	197. BD* (1) O 19- C 29	0.65	0.52	0.016
62. LP (1) Sb 14	204. BD* (1) O 24- C 34	0.62	0.66	0.018
62. LP (1) Sb 14	205. BD* (1) O 25- C 33	0.74	0.50	0.017
62. LP (1) Sb 14	575. RY (1) Sb 14	1.16	1.82	0.041

62. LP (1)Sb 14	586. RY (12)Sb 14	1.29	2.00	0.045
62. LP (1)Sb 14	589. RY (15)Sb 14	2.16	1.63	0.053
62. LP (1)Sb 14	590. RY (16)Sb 14	1.01	2.19	0.042
62. LP (1)Sb 14	691. RY (2) O 18	0.92	1.67	0.035
62. LP (1)Sb 14	717. RY (2) O 19	0.66	1.60	0.029
62. LP (1)Sb 14	848. RY (3) O 24	0.54	1.58	0.026
62. LP (1)Sb 14	872. RY (1) O 25	0.55	1.71	0.027
63. LP (1) O 15	188. BD* (1)Sb 13- O 21	1.21	0.84	0.028
63. LP (1) O 15	189. BD* (1)Sb 13- O 22	4.34	0.82	0.053
63. LP (1) O 15	192. BD* (1) O 15- C 27	0.66	1.05	0.023
63. LP (1) O 15	208. BD* (1) C 27- C 28	5.05	0.97	0.063
63. LP (1) O 15	614. RY (3) O 15	19.53	1.89	0.171
63. LP (1) O 15	616. RY (5) O 15	0.80	2.40	0.039
63. LP (1) O 15	621. RY (10) O 15	1.40	5.02	0.075
63. LP (1) O 15	624. RY (13) O 15	1.43	4.80	0.074
63. LP (1) O 15	628. RY (17) O 15	1.38	22.93	0.159
63. LP (1) O 15	630. RY (19) O 15	1.31	9.78	0.101
63. LP (1) O 15	632. RY (21) O 15	0.52	7.67	0.056
63. LP (1) O 15	924. RY (1) C 27	0.66	1.96	0.032
63. LP (1) O 15	925. RY (2) C 27	0.85	2.33	0.040
63. LP (1) O 15	931. RY (8) C 27	0.75	2.87	0.041
64. LP (2) O 15	188. BD* (1)Sb 13- O 21	0.92	0.56	0.020
64. LP (2) O 15	208. BD* (1) C 27- C 28	1.32	0.69	0.027
64. LP (2) O 15	209. BD* (1) C 27- H 57	7.07	0.76	0.065
64. LP (2) O 15	612. RY (1) O 15	26.78	1.47	0.177
64. LP (2) O 15	615. RY (4) O 15	1.79	2.47	0.059
64. LP (2) O 15	626. RY (15) O 15	0.94	5.85	0.066
64. LP (2) O 15	637. RY (26) O 15	0.80	6.15	0.063
64. LP (2) O 15	926. RY (3) C 27	1.06	2.34	0.044
64. LP (2) O 15	927. RY (4) C 27	1.35	1.78	0.044
64. LP (2) O 15	937. RY (14) C 27	0.56	2.99	0.037
65. LP (3) O 15	187. BD* (1)Sb 13- O 16	6.96	0.67	0.061
65. LP (3) O 15	188. BD* (1)Sb 13- O 21	7.37	0.68	0.063
65. LP (3) O 15	189. BD* (1)Sb 13- O 22	16.76	0.66	0.094
65. LP (3) O 15	194. BD* (1) O 17- C 27	16.99	0.89	0.110
65. LP (3) O 15	208. BD* (1) C 27- C 28	3.48	0.81	0.047
65. LP (3) O 15	209. BD* (1) C 27- H 57	0.70	0.88	0.022
65. LP (3) O 15	538. RY (1)Sb 13	5.18	1.89	0.088
65. LP (3) O 15	540. RY (3)Sb 13	0.74	1.96	0.034
65. LP (3) O 15	543. RY (6)Sb 13	0.70	1.77	0.032
65. LP (3) O 15	549. RY (12)Sb 13	1.32	1.84	0.044
65. LP (3) O 15	551. RY (14)Sb 13	1.47	1.88	0.047
65. LP (3) O 15	555. RY (18)Sb 13	2.59	2.54	0.072
65. LP (3) O 15	558. RY (21)Sb 13	0.77	2.65	0.040
65. LP (3) O 15	560. RY (23)Sb 13	0.78	2.64	0.040
65. LP (3) O 15	569. RY (32)Sb 13	2.41	51.17	0.313
65. LP (3) O 15	572. RY (35)Sb 13	0.51	4.38	0.042
65. LP (3) O 15	613. RY (2) O 15	15.90	1.78	0.150
65. LP (3) O 15	614. RY (3) O 15	0.74	1.72	0.032
65. LP (3) O 15	623. RY (12) O 15	0.52	5.03	0.046
65. LP (3) O 15	625. RY (14) O 15	1.57	5.01	0.079
65. LP (3) O 15	628. RY (17) O 15	0.82	22.77	0.122
65. LP (3) O 15	629. RY (18) O 15	0.72	10.18	0.076
65. LP (3) O 15	924. RY (1) C 27	2.77	1.80	0.063
65. LP (3) O 15	925. RY (2) C 27	2.03	2.17	0.059
65. LP (3) O 15	929. RY (6) C 27	0.64	3.60	0.043
65. LP (3) O 15	938. RY (15) C 27	0.61	3.02	0.038
66. LP (1) O 16	193. BD* (1) O 16- C 28	1.23	0.86	0.029
66. LP (1) O 16	208. BD* (1) C 27- C 28	1.73	0.99	0.037
66. LP (1) O 16	544. RY (7)Sb 13	0.93	2.02	0.039
66. LP (1) O 16	638. RY (1) O 16	2.86	1.98	0.067
66. LP (1) O 16	639. RY (2) O 16	6.12	1.85	0.095
66. LP (1) O 16	640. RY (3) O 16	8.78	2.06	0.120
66. LP (1) O 16	641. RY (4) O 16	0.64	2.34	0.035
66. LP (1) O 16	643. RY (6) O 16	0.53	3.10	0.036
66. LP (1) O 16	651. RY (14) O 16	1.34	5.77	0.079
66. LP (1) O 16	653. RY (16) O 16	1.20	36.02	0.186
66. LP (1) O 16	663. RY (26) O 16	1.23	5.40	0.073
66. LP (1) O 16	951. RY (2) C 28	0.50	1.98	0.028
66. LP (1) O 16	955. RY (6) C 28	0.69	2.92	0.040
67. LP (2) O 16	188. BD* (1)Sb 13- O 21	1.09	0.57	0.022
67. LP (2) O 16	210. BD* (1) C 28- C 29	2.29	0.71	0.036
67. LP (2) O 16	211. BD* (1) C 28- H 58	3.09	0.83	0.045
67. LP (2) O 16	539. RY (2)Sb 13	0.84	1.82	0.035
67. LP (2) O 16	542. RY (5)Sb 13	0.72	1.62	0.031
67. LP (2) O 16	638. RY (1) O 16	14.69	1.69	0.141
67. LP (2) O 16	639. RY (2) O 16	10.69	1.56	0.115
67. LP (2) O 16	650. RY (13) O 16	0.90	5.16	0.061
67. LP (2) O 16	652. RY (15) O 16	1.04	5.62	0.068
67. LP (2) O 16	661. RY (24) O 16	0.91	5.98	0.066
67. LP (2) O 16	952. RY (3) C 28	2.05	1.84	0.055
68. LP (1) O 17	192. BD* (1) O 15- C 27	1.46	1.03	0.035
68. LP (1) O 17	208. BD* (1) C 27- C 28	5.77	0.96	0.066
68. LP (1) O 17	665. RY (2) O 17	12.56	1.91	0.138
68. LP (1) O 17	666. RY (3) O 17	4.21	2.91	0.099
68. LP (1) O 17	668. RY (5) O 17	2.38	2.65	0.071
68. LP (1) O 17	670. RY (7) O 17	0.80	3.76	0.049
68. LP (1) O 17	671. RY (8) O 17	0.91	3.33	0.049
68. LP (1) O 17	673. RY (10) O 17	1.54	4.36	0.073
68. LP (1) O 17	683. RY (20) O 17	0.78	15.32	0.098
68. LP (1) O 17	684. RY (21) O 17	0.71	12.01	0.083
68. LP (1) O 17	688. RY (25) O 17	1.02	10.09	0.091
68. LP (1) O 17	924. RY (1) C 27	0.61	1.95	0.031
68. LP (1) O 17	925. RY (2) C 27	0.76	2.32	0.037
68. LP (1) O 17	934. RY (11) C 27	0.73	2.50	0.038
69. LP (2) O 17	192. BD* (1) O 15- C 27	0.85	0.83	0.024
69. LP (2) O 17	209. BD* (1) C 27- H 57	7.64	0.83	0.071
69. LP (2) O 17	664. RY (1) O 17	23.93	1.53	0.171
69. LP (2) O 17	665. RY (2) O 17	0.81	1.70	0.033
69. LP (2) O 17	666. RY (3) O 17	1.65	2.71	0.060
69. LP (2) O 17	667. RY (4) O 17	2.29	2.60	0.069
69. LP (2) O 17	668. RY (5) O 17	0.87	2.45	0.041
69. LP (2) O 17	669. RY (6) O 17	1.11	2.32	0.045

69. LP (2) O 17	675. RY (12) O 17	1.73	3.65	0.071
69. LP (2) O 17	676. RY (13) O 17	0.50	8.49	0.058
69. LP (2) O 17	927. RY (4) C 27	1.16	1.85	0.041
69. LP (2) O 17	935. RY (12) C 27	1.00	3.30	0.051
69. LP (2) O 17	1223. RY (2) H 53	1.14	2.51	0.048
70. LP (1) O 18	156. LV (1) Sb 14	5.93	0.83	0.063
70. LP (1) O 18	212. BD* (1) C 29- C 30	3.85	0.99	0.055
70. LP (1) O 18	691. RY (2) O 18	4.28	2.06	0.084
70. LP (1) O 18	692. RY (3) O 18	13.97	1.92	0.146
70. LP (1) O 18	700. RY (11) O 18	0.66	5.85	0.056
70. LP (1) O 18	701. RY (12) O 18	0.61	5.16	0.050
70. LP (1) O 18	702. RY (13) O 18	1.61	4.83	0.079
70. LP (1) O 18	703. RY (14) O 18	0.75	5.77	0.059
70. LP (1) O 18	704. RY (15) O 18	1.29	30.29	0.177
70. LP (1) O 18	706. RY (17) O 18	0.56	10.89	0.070
70. LP (1) O 18	715. RY (26) O 18	0.73	5.29	0.056
70. LP (1) O 18	1003. RY (2) C 30	0.92	2.35	0.041
70. LP (1) O 18	1009. RY (8) C 30	0.58	3.11	0.038
70. LP (1) O 18	1013. RY (12) C 30	0.57	2.59	0.034
71. LP (2) O 18	156. LV (1) Sb 14	11.89	0.55	0.073
71. LP (2) O 18	190. BD* (1) Sb 14- O 19	2.99	0.60	0.038
71. LP (2) O 18	191. BD* (1) Sb 14- O 25	2.20	0.61	0.033
71. LP (2) O 18	198. BD* (1) O 20- C 30	9.35	0.84	0.079
71. LP (2) O 18	212. BD* (1) C 29- C 30	0.61	0.72	0.019
71. LP (2) O 18	214. BD* (1) C 30- H 60	2.95	0.83	0.044
71. LP (2) O 18	577. RY (3) Sb 14	0.58	1.99	0.030
71. LP (2) O 18	578. RY (4) Sb 14	1.00	1.48	0.034
71. LP (2) O 18	584. RY (10) Sb 14	0.98	1.84	0.038
71. LP (2) O 18	593. RY (19) Sb 14	0.56	2.39	0.033
71. LP (2) O 18	595. RY (21) Sb 14	0.56	2.14	0.031
71. LP (2) O 18	604. RY (30) Sb 14	0.77	14.53	0.094
71. LP (2) O 18	610. RY (36) Sb 14	0.81	18.69	0.110
71. LP (2) O 18	611. RY (37) Sb 14	0.77	16.17	0.099
71. LP (2) O 18	690. RY (1) O 18	22.54	1.53	0.166
71. LP (2) O 18	691. RY (2) O 18	0.95	1.79	0.037
71. LP (2) O 18	692. RY (3) O 18	1.53	1.65	0.045
71. LP (2) O 18	701. RY (12) O 18	0.55	4.89	0.046
71. LP (2) O 18	702. RY (13) O 18	0.68	4.56	0.050
71. LP (2) O 18	703. RY (14) O 18	1.25	5.49	0.074
71. LP (2) O 18	714. RY (25) O 18	0.67	6.30	0.058
71. LP (2) O 18	1002. RY (1) C 30	0.73	1.77	0.032
71. LP (2) O 18	1003. RY (2) C 30	1.60	2.08	0.051
72. LP (3) O 18	156. LV (1) Sb 14	18.34	0.59	0.093
72. LP (3) O 18	190. BD* (1) Sb 14- O 19	4.67	0.64	0.049
72. LP (3) O 18	191. BD* (1) Sb 14- O 25	0.94	0.65	0.022
72. LP (3) O 18	198. BD* (1) O 20- C 30	5.25	0.88	0.061
72. LP (3) O 18	212. BD* (1) C 29- C 30	2.84	0.76	0.041
72. LP (3) O 18	214. BD* (1) C 30- H 60	1.62	0.87	0.033
72. LP (3) O 18	576. RY (2) Sb 14	1.33	2.16	0.048
72. LP (3) O 18	577. RY (3) Sb 14	0.74	2.03	0.035
72. LP (3) O 18	589. RY (15) Sb 14	0.67	1.79	0.031
72. LP (3) O 18	593. RY (19) Sb 14	0.65	2.43	0.035
72. LP (3) O 18	594. RY (20) Sb 14	0.82	2.93	0.044
72. LP (3) O 18	595. RY (21) Sb 14	0.51	2.18	0.030
72. LP (3) O 18	596. RY (22) Sb 14	0.74	2.47	0.038
72. LP (3) O 18	604. RY (30) Sb 14	0.99	14.57	0.107
72. LP (3) O 18	609. RY (35) Sb 14	0.65	13.80	0.085
72. LP (3) O 18	610. RY (36) Sb 14	1.21	18.72	0.134
72. LP (3) O 18	611. RY (37) Sb 14	1.06	16.20	0.117
72. LP (3) O 18	690. RY (1) O 18	5.55	1.57	0.083
72. LP (3) O 18	691. RY (2) O 18	6.91	1.83	0.100
72. LP (3) O 18	692. RY (3) O 18	5.66	1.68	0.087
72. LP (3) O 18	693. RY (4) O 18	0.58	2.89	0.036
72. LP (3) O 18	702. RY (13) O 18	0.75	4.59	0.052
72. LP (3) O 18	704. RY (15) O 18	0.70	30.05	0.129
72. LP (3) O 18	715. RY (26) O 18	1.48	5.06	0.077
72. LP (3) O 18	1002. RY (1) C 30	0.61	1.81	0.030
72. LP (3) O 18	1003. RY (2) C 30	1.10	2.11	0.043
72. LP (3) O 18	1004. RY (3) C 30	0.84	2.32	0.039
73. LP (1) O 19	156. LV (1) Sb 14	1.02	0.79	0.025
73. LP (1) O 19	197. BD* (1) O 19- C 29	1.06	0.88	0.027
73. LP (1) O 19	212. BD* (1) C 29- C 30	2.64	0.96	0.045
73. LP (1) O 19	579. RY (5) Sb 14	0.68	2.07	0.034
73. LP (1) O 19	716. RY (1) O 19	3.82	2.01	0.078
73. LP (1) O 19	717. RY (2) O 19	5.42	1.96	0.092
73. LP (1) O 19	718. RY (3) O 19	8.80	2.11	0.122
73. LP (1) O 19	729. RY (14) O 19	2.73	4.93	0.103
73. LP (1) O 19	731. RY (16) O 19	1.20	35.13	0.183
73. LP (1) O 19	978. RY (3) C 29	0.55	2.18	0.031
73. LP (1) O 19	979. RY (4) C 29	0.80	2.27	0.038
73. LP (1) O 19	982. RY (7) C 29	0.80	2.53	0.040
74. LP (2) O 19	191. BD* (1) Sb 14- O 25	0.99	0.59	0.021
74. LP (2) O 19	210. BD* (1) C 28- C 29	3.69	0.71	0.046
74. LP (2) O 19	213. BD* (1) C 29- H 59	3.91	0.83	0.051
74. LP (2) O 19	575. RY (1) Sb 14	1.38	1.91	0.046
74. LP (2) O 19	580. RY (6) Sb 14	0.86	1.77	0.035
74. LP (2) O 19	716. RY (1) O 19	14.56	1.75	0.142
74. LP (2) O 19	717. RY (2) O 19	9.27	1.70	0.112
74. LP (2) O 19	728. RY (13) O 19	0.81	4.94	0.057
74. LP (2) O 19	736. RY (21) O 19	0.54	5.92	0.050
74. LP (2) O 19	741. RY (26) O 19	2.16	5.08	0.094
74. LP (2) O 19	977. RY (2) C 29	0.69	1.74	0.031
74. LP (2) O 19	979. RY (4) C 29	1.34	2.01	0.046
74. LP (2) O 19	981. RY (6) C 29	0.63	2.31	0.034
75. LP (1) O 20	196. BD* (1) O 18- C 30	1.71	0.97	0.036
75. LP (1) O 20	212. BD* (1) C 29- C 30	6.78	0.96	0.072
75. LP (1) O 20	743. RY (2) O 20	11.10	1.93	0.131
75. LP (1) O 20	744. RY (3) O 20	6.80	2.53	0.117
75. LP (1) O 20	746. RY (5) O 20	2.32	2.61	0.069
75. LP (1) O 20	750. RY (9) O 20	2.94	3.28	0.088
75. LP (1) O 20	757. RY (16) O 20	0.80	6.09	0.062
75. LP (1) O 20	759. RY (18) O 20	0.61	11.14	0.074
75. LP (1) O 20	761. RY (20) O 20	0.87	12.58	0.093

75. LP (1) O 20	762. RY (21) O 20	0.68	11.88	0.080
75. LP (1) O 20	766. RY (25) O 20	0.72	14.01	0.090
75. LP (1) O 20	1002. RY (1) C 30	1.51	2.01	0.049
75. LP (1) O 20	1003. RY (2) C 30	0.66	2.32	0.035
76. LP (2) O 20	196. BD*(1) O 18- C 30	1.02	0.77	0.025
76. LP (2) O 20	212. BD*(1) C 29- C 30	0.52	0.76	0.018
76. LP (2) O 20	214. BD*(1) C 30- H 60	6.41	0.87	0.067
76. LP (2) O 20	742. RY (1) O 20	25.98	1.56	0.179
76. LP (2) O 20	743. RY (2) O 20	1.12	1.73	0.039
76. LP (2) O 20	744. RY (3) O 20	2.23	2.33	0.064
76. LP (2) O 20	745. RY (4) O 20	1.04	2.67	0.047
76. LP (2) O 20	747. RY (6) O 20	0.96	2.82	0.047
76. LP (2) O 20	749. RY (8) O 20	0.81	2.99	0.044
76. LP (2) O 20	753. RY (12) O 20	1.70	3.64	0.070
76. LP (2) O 20	755. RY (14) O 20	0.55	7.80	0.059
76. LP (2) O 20	757. RY (16) O 20	0.55	5.89	0.051
76. LP (2) O 20	1004. RY (3) C 30	0.60	2.32	0.033
76. LP (2) O 20	1228. RY (2) H 54	0.81	2.60	0.041
77. LP (1) O 21	200. BD*(1) O 21- C 32	1.17	0.85	0.028
77. LP (1) O 21	215. BD*(1) C 31- C 32	1.66	1.00	0.036
77. LP (1) O 21	542. RY (5) Sb 13	0.63	1.90	0.031
77. LP (1) O 21	545. RY (8) Sb 13	0.67	2.05	0.033
77. LP (1) O 21	768. RY (1) O 21	3.61	2.00	0.076
77. LP (1) O 21	769. RY (2) O 21	4.28	1.90	0.080
77. LP (1) O 21	770. RY (3) O 21	9.96	2.04	0.127
77. LP (1) O 21	782. RY (15) O 21	3.59	4.60	0.115
77. LP (1) O 21	783. RY (16) O 21	1.13	32.32	0.171
77. LP (1) O 21	793. RY (26) O 21	0.59	8.32	0.062
77. LP (1) O 21	1057. RY (4) C 32	0.89	2.34	0.041
77. LP (1) O 21	1060. RY (7) C 32	0.92	2.64	0.044
78. LP (2) O 21	187. BD*(1) Sb 13- O 16	1.13	0.56	0.022
78. LP (2) O 21	217. BD*(1) C 32- C 33	2.59	0.69	0.038
78. LP (2) O 21	218. BD*(1) C 32- H 62	3.04	0.82	0.045
78. LP (2) O 21	539. RY (2) Sb 13	0.97	1.82	0.037
78. LP (2) O 21	543. RY (6) Sb 13	0.57	1.65	0.028
78. LP (2) O 21	768. RY (1) O 21	13.89	1.71	0.137
78. LP (2) O 21	769. RY (2) O 21	11.14	1.61	0.119
78. LP (2) O 21	781. RY (14) O 21	3.04	4.74	0.107
78. LP (2) O 21	1057. RY (4) C 32	1.33	2.05	0.047
78. LP (2) O 21	1059. RY (6) C 32	0.57	2.22	0.032
79. LP (1) O 22	189. BD*(1) Sb 13- O 22	1.43	0.85	0.031
79. LP (1) O 22	201. BD*(1) O 22- C 31	0.99	1.02	0.028
79. LP (1) O 22	215. BD*(1) C 31- C 32	4.76	1.01	0.062
79. LP (1) O 22	795. RY (2) O 22	0.66	1.96	0.032
79. LP (1) O 22	796. RY (3) O 22	19.23	1.90	0.171
79. LP (1) O 22	798. RY (5) O 22	0.62	2.43	0.035
79. LP (1) O 22	802. RY (9) O 22	0.82	2.98	0.044
79. LP (1) O 22	805. RY (12) O 22	2.20	4.57	0.090
79. LP (1) O 22	810. RY (17) O 22	1.45	24.72	0.169
79. LP (1) O 22	811. RY (18) O 22	1.17	16.25	0.123
79. LP (1) O 22	814. RY (21) O 22	0.72	6.97	0.063
79. LP (1) O 22	1029. RY (2) C 31	0.85	2.35	0.040
80. LP (2) O 22	187. BD*(1) Sb 13- O 16	2.80	0.61	0.037
80. LP (2) O 22	188. BD*(1) Sb 13- O 21	0.99	0.61	0.022
80. LP (2) O 22	189. BD*(1) Sb 13- O 22	10.29	0.59	0.070
80. LP (2) O 22	202. BD*(1) O 23- C 31	10.31	0.85	0.084
80. LP (2) O 22	215. BD*(1) C 31- C 32	0.67	0.75	0.020
80. LP (2) O 22	216. BD*(1) C 31- H 61	3.05	0.84	0.045
80. LP (2) O 22	540. RY (3) Sb 13	1.07	1.90	0.040
80. LP (2) O 22	541. RY (4) Sb 13	1.27	1.54	0.040
80. LP (2) O 22	550. RY (13) Sb 13	0.77	1.74	0.033
80. LP (2) O 22	555. RY (18) Sb 13	1.01	2.47	0.045
80. LP (2) O 22	560. RY (23) Sb 13	0.55	2.58	0.034
80. LP (2) O 22	569. RY (32) Sb 13	1.14	51.10	0.215
80. LP (2) O 22	794. RY (1) O 22	22.49	1.51	0.165
80. LP (2) O 22	795. RY (2) O 22	3.01	1.70	0.064
80. LP (2) O 22	796. RY (3) O 22	1.02	1.64	0.037
80. LP (2) O 22	806. RY (13) O 22	1.26	5.37	0.073
80. LP (2) O 22	819. RY (26) O 22	1.09	5.18	0.067
80. LP (2) O 22	1028. RY (1) C 31	1.07	1.77	0.039
80. LP (2) O 22	1029. RY (2) C 31	1.42	2.10	0.049
81. LP (1) O 23	201. BD*(1) O 22- C 31	1.93	0.99	0.039
81. LP (1) O 23	215. BD*(1) C 31- C 32	6.75	0.98	0.073
81. LP (1) O 23	821. RY (2) O 23	10.70	1.92	0.128
81. LP (1) O 23	822. RY (3) O 23	7.28	2.54	0.121
81. LP (1) O 23	824. RY (5) O 23	2.51	2.50	0.071
81. LP (1) O 23	827. RY (8) O 23	0.54	3.16	0.037
81. LP (1) O 23	828. RY (9) O 23	0.82	3.81	0.050
81. LP (1) O 23	830. RY (11) O 23	1.18	3.81	0.060
81. LP (1) O 23	834. RY (15) O 23	0.60	5.35	0.050
81. LP (1) O 23	838. RY (19) O 23	1.15	19.77	0.135
81. LP (1) O 23	843. RY (24) O 23	1.05	14.50	0.110
81. LP (1) O 23	1028. RY (1) C 31	1.24	2.00	0.044
81. LP (1) O 23	1029. RY (2) C 31	0.81	2.33	0.039
81. LP (1) O 23	1044. RY (17) C 31	0.70	2.60	0.038
82. LP (2) O 23	215. BD*(1) C 31- C 32	1.10	0.78	0.026
82. LP (2) O 23	216. BD*(1) C 31- H 61	6.37	0.87	0.066
82. LP (2) O 23	820. RY (1) O 23	27.69	1.52	0.183
82. LP (2) O 23	821. RY (2) O 23	0.94	1.72	0.036
82. LP (2) O 23	822. RY (3) O 23	1.74	2.34	0.057
82. LP (2) O 23	823. RY (4) O 23	1.08	2.50	0.046
82. LP (2) O 23	828. RY (9) O 23	1.64	3.61	0.069
82. LP (2) O 23	830. RY (11) O 23	1.05	3.61	0.055
82. LP (2) O 23	1030. RY (3) C 31	0.70	2.30	0.036
82. LP (2) O 23	1232. RY (1) H 55	0.53	1.66	0.027
82. LP (2) O 23	1233. RY (2) H 55	0.74	2.65	0.040
83. LP (1) O 24	156. LV (1) Sb 14	6.24	0.80	0.063
83. LP (1) O 24	204. BD*(1) O 24- C 34	0.64	1.02	0.023
83. LP (1) O 24	219. BD*(1) C 33- C 34	4.59	0.97	0.060
83. LP (1) O 24	847. RY (2) O 24	0.68	1.95	0.033
83. LP (1) O 24	848. RY (3) O 24	18.12	1.95	0.168
83. LP (1) O 24	850. RY (5) O 24	0.75	2.57	0.039
83. LP (1) O 24	855. RY (10) O 24	1.05	5.30	0.067

83. LP (1) O 24	857. RY (12) O 24	1.48	4.62	0.074
83. LP (1) O 24	859. RY (14) O 24	1.20	5.32	0.071
83. LP (1) O 24	862. RY (17) O 24	1.33	32.85	0.187
83. LP (1) O 24	864. RY (19) O 24	0.78	7.26	0.067
83. LP (1) O 24	868. RY (23) O 24	0.64	10.15	0.072
83. LP (1) O 24	1107. RY (2) C 34	0.71	2.31	0.036
83. LP (1) O 24	1113. RY (8) C 34	0.82	2.94	0.044
84. LP (2) O 24	190. BD* (1) Sb 14- O 19	0.62	0.55	0.016
84. LP (2) O 24	219. BD* (1) C 33- C 34	0.75	0.68	0.020
84. LP (2) O 24	221. BD* (1) C 34- H 64	7.14	0.75	0.065
84. LP (2) O 24	846. RY (1) O 24	26.95	1.47	0.178
84. LP (2) O 24	847. RY (2) O 24	0.80	1.66	0.033
84. LP (2) O 24	849. RY (4) O 24	1.24	2.51	0.050
84. LP (2) O 24	860. RY (15) O 24	2.01	5.02	0.090
84. LP (2) O 24	1108. RY (3) C 34	0.98	2.27	0.042
84. LP (2) O 24	1109. RY (4) C 34	1.19	1.73	0.041
84. LP (2) O 24	1119. RY (14) C 34	0.63	3.46	0.042
85. LP (3) O 24	156. LV (1) Sb 14	30.05	0.64	0.123
85. LP (3) O 24	190. BD* (1) Sb 14- O 19	2.81	0.68	0.039
85. LP (3) O 24	191. BD* (1) Sb 14- O 25	7.50	0.70	0.064
85. LP (3) O 24	206. BD* (1) O 26- C 34	14.95	0.91	0.104
85. LP (3) O 24	219. BD* (1) C 33- C 34	3.16	0.81	0.045
85. LP (3) O 24	576. RY (2) Sb 14	2.13	2.21	0.061
85. LP (3) O 24	577. RY (3) Sb 14	1.56	2.08	0.051
85. LP (3) O 24	578. RY (4) Sb 14	0.73	1.56	0.030
85. LP (3) O 24	588. RY (14) Sb 14	1.81	1.85	0.052
85. LP (3) O 24	589. RY (15) Sb 14	1.19	1.83	0.042
85. LP (3) O 24	593. RY (19) Sb 14	0.54	2.47	0.033
85. LP (3) O 24	594. RY (20) Sb 14	1.66	2.97	0.063
85. LP (3) O 24	595. RY (21) Sb 14	0.50	2.22	0.030
85. LP (3) O 24	600. RY (26) Sb 14	0.95	4.10	0.056
85. LP (3) O 24	602. RY (28) Sb 14	0.58	4.95	0.048
85. LP (3) O 24	604. RY (30) Sb 14	1.98	14.61	0.152
85. LP (3) O 24	609. RY (35) Sb 14	0.72	13.84	0.089
85. LP (3) O 24	610. RY (36) Sb 14	2.39	18.77	0.189
85. LP (3) O 24	611. RY (37) Sb 14	2.36	16.25	0.175
85. LP (3) O 24	846. RY (1) O 24	0.62	1.60	0.028
85. LP (3) O 24	847. RY (2) O 24	15.80	1.79	0.150
85. LP (3) O 24	857. RY (12) O 24	0.58	4.46	0.045
85. LP (3) O 24	858. RY (13) O 24	0.53	5.01	0.046
85. LP (3) O 24	859. RY (14) O 24	1.13	5.16	0.068
85. LP (3) O 24	862. RY (17) O 24	1.01	32.69	0.162
85. LP (3) O 24	1106. RY (1) C 34	1.91	1.82	0.053
85. LP (3) O 24	1107. RY (2) C 34	2.42	2.15	0.064
85. LP (3) O 24	1111. RY (6) C 34	0.54	3.60	0.039
85. LP (3) O 24	1120. RY (15) C 34	0.67	2.72	0.038
86. LP (1) O 25	156. LV (1) Sb 14	0.81	0.80	0.023
86. LP (1) O 25	205. BD* (1) O 25- C 33	1.06	0.87	0.027
86. LP (1) O 25	219. BD* (1) C 33- C 34	2.34	0.98	0.043
86. LP (1) O 25	580. RY (6) Sb 14	0.52	2.05	0.029
86. LP (1) O 25	581. RY (7) Sb 14	0.52	2.09	0.029
86. LP (1) O 25	872. RY (1) O 25	1.81	2.08	0.055
86. LP (1) O 25	873. RY (2) O 25	7.89	1.94	0.110
86. LP (1) O 25	874. RY (3) O 25	6.89	2.23	0.111
86. LP (1) O 25	875. RY (4) O 25	0.65	2.38	0.035
86. LP (1) O 25	886. RY (15) O 25	1.07	5.96	0.071
86. LP (1) O 25	896. RY (25) O 25	1.25	5.68	0.075
86. LP (1) O 25	897. RY (26) O 25	1.20	35.74	0.185
86. LP (1) O 25	1081. RY (2) C 33	0.67	1.97	0.032
86. LP (1) O 25	1082. RY (3) C 33	0.72	2.18	0.035
86. LP (1) O 25	1085. RY (6) C 33	0.54	2.62	0.033
86. LP (1) O 25	1086. RY (7) C 33	0.62	2.80	0.037
87. LP (2) O 25	190. BD* (1) Sb 14- O 19	1.11	0.59	0.023
87. LP (2) O 25	217. BD* (1) C 32- C 33	2.70	0.71	0.039
87. LP (2) O 25	220. BD* (1) C 33- H 63	3.43	0.85	0.048
87. LP (2) O 25	575. RY (1) Sb 14	0.63	1.93	0.031
87. LP (2) O 25	579. RY (5) Sb 14	1.18	1.82	0.041
87. LP (2) O 25	872. RY (1) O 25	13.63	1.81	0.140
87. LP (2) O 25	873. RY (2) O 25	7.53	1.67	0.100
87. LP (2) O 25	884. RY (13) O 25	1.12	5.01	0.067
87. LP (2) O 25	885. RY (14) O 25	1.32	5.56	0.076
87. LP (2) O 25	1081. RY (2) C 33	0.68	1.70	0.030
87. LP (2) O 25	1082. RY (3) C 33	1.63	1.91	0.050
88. LP (1) O 26	204. BD* (1) O 24- C 34	1.83	1.01	0.038
88. LP (1) O 26	219. BD* (1) C 33- C 34	6.45	0.96	0.070
88. LP (1) O 26	899. RY (2) O 26	11.66	1.91	0.133
88. LP (1) O 26	900. RY (3) O 26	4.50	2.89	0.102
88. LP (1) O 26	902. RY (5) O 26	2.30	2.68	0.070
88. LP (1) O 26	904. RY (7) O 26	0.63	3.64	0.043
88. LP (1) O 26	906. RY (9) O 26	0.86	3.69	0.050
88. LP (1) O 26	907. RY (10) O 26	1.40	3.69	0.064
88. LP (1) O 26	910. RY (13) O 26	0.88	4.33	0.055
88. LP (1) O 26	915. RY (18) O 26	0.57	9.89	0.067
88. LP (1) O 26	918. RY (21) O 26	1.29	15.97	0.128
88. LP (1) O 26	922. RY (25) O 26	0.67	9.95	0.073
88. LP (1) O 26	1106. RY (1) C 34	1.02	1.97	0.040
88. LP (1) O 26	1108. RY (3) C 34	0.57	2.55	0.034
88. LP (1) O 26	1116. RY (11) C 34	0.66	2.70	0.038
89. LP (2) O 26	219. BD* (1) C 33- C 34	0.78	0.76	0.022
89. LP (2) O 26	221. BD* (1) C 34- H 64	7.55	0.83	0.071
89. LP (2) O 26	898. RY (1) O 26	24.18	1.52	0.171
89. LP (2) O 26	899. RY (2) O 26	0.82	1.71	0.033
89. LP (2) O 26	900. RY (3) O 26	1.53	2.69	0.057
89. LP (2) O 26	901. RY (4) O 26	2.34	2.52	0.068
89. LP (2) O 26	902. RY (5) O 26	0.70	2.48	0.037
89. LP (2) O 26	903. RY (6) O 26	0.75	2.28	0.037
89. LP (2) O 26	909. RY (12) O 26	2.25	3.91	0.084
89. LP (2) O 26	1109. RY (4) C 34	1.53	1.81	0.047
89. LP (2) O 26	1117. RY (12) C 34	0.64	3.11	0.040
89. LP (2) O 26	1238. RY (2) H 56	1.14	2.53	0.048
120. BD (1) Sb 13- O 16	187. BD* (1) Sb 13- O 16	15.13	0.79	0.098
120. BD (1) Sb 13- O 16	188. BD* (1) Sb 13- O 21	1.41	0.80	0.030
120. BD (1) Sb 13- O 16	193. BD* (1) O 16- C 28	0.66	0.79	0.020

120.	BD	(1)Sb	13-	O	16	208.	BD*	(1) C	27-	C	28	0.94	0.93	0.026
120.	BD	(1)Sb	13-	O	16	210.	BD*	(1) C	28-	C	29	1.70	0.94	0.036
120.	BD	(1)Sb	13-	O	16	559.	RY	(22)Sb	13			0.51	2.97	0.035
120.	BD	(1)Sb	13-	O	16	638.	RY	(1) O	16			1.29	1.91	0.044
120.	BD	(1)Sb	13-	O	16	639.	RY	(2) O	16			2.03	1.79	0.054
120.	BD	(1)Sb	13-	O	16	640.	RY	(3) O	16			4.27	1.99	0.082
120.	BD	(1)Sb	13-	O	16	649.	RY	(12) O	16			0.59	4.99	0.049
120.	BD	(1)Sb	13-	O	16	950.	RY	(1) C	28			0.75	1.72	0.032
120.	BD	(1)Sb	13-	O	16	952.	RY	(3) C	28			1.16	2.06	0.044
120.	BD	(1)Sb	13-	O	16	1257.	RY	(1) H	60			0.84	2.36	0.040
121.	BD	(1)Sb	13-	O	21	187.	BD*	(1)Sb	13-	O	16	1.59	0.79	0.032
121.	BD	(1)Sb	13-	O	21	188.	BD*	(1)Sb	13-	O	21	14.66	0.79	0.096
121.	BD	(1)Sb	13-	O	21	189.	BD*	(1)Sb	13-	O	22	2.86	0.78	0.042
121.	BD	(1)Sb	13-	O	21	200.	BD*	(1) O	21-	C	32	0.65	0.79	0.020
121.	BD	(1)Sb	13-	O	21	215.	BD*	(1) C	31-	C	32	0.80	0.94	0.024
121.	BD	(1)Sb	13-	O	21	217.	BD*	(1) C	32-	C	33	1.01	0.92	0.027
121.	BD	(1)Sb	13-	O	21	559.	RY	(22)Sb	13			0.89	2.97	0.046
121.	BD	(1)Sb	13-	O	21	768.	RY	(1) O	21			0.98	1.94	0.039
121.	BD	(1)Sb	13-	O	21	769.	RY	(2) O	21			1.79	1.84	0.051
121.	BD	(1)Sb	13-	O	21	770.	RY	(3) O	21			3.25	1.98	0.072
121.	BD	(1)Sb	13-	O	21	771.	RY	(4) O	21			0.99	2.06	0.040
121.	BD	(1)Sb	13-	O	21	775.	RY	(8) O	21			0.56	4.51	0.045
121.	BD	(1)Sb	13-	O	21	779.	RY	(12) O	21			0.53	5.13	0.047
121.	BD	(1)Sb	13-	O	21	1054.	RY	(1) C	32			3.14	1.91	0.069
122.	BD	(1)Sb	13-	O	22	187.	BD*	(1)Sb	13-	O	16	0.63	0.61	0.017
122.	BD	(1)Sb	13-	O	22	188.	BD*	(1)Sb	13-	O	21	1.17	0.62	0.024
122.	BD	(1)Sb	13-	O	22	189.	BD*	(1)Sb	13-	O	22	8.47	0.60	0.064
122.	BD	(1)Sb	13-	O	22	201.	BD*	(1) O	22-	C	31	1.88	0.77	0.034
122.	BD	(1)Sb	13-	O	22	202.	BD*	(1) O	23-	C	31	4.14	0.86	0.053
122.	BD	(1)Sb	13-	O	22	215.	BD*	(1) C	31-	C	32	2.86	0.76	0.042
122.	BD	(1)Sb	13-	O	22	216.	BD*	(1) C	31-	H	61	3.04	0.84	0.045
122.	BD	(1)Sb	13-	O	22	543.	RY	(6)Sb	13			0.72	1.71	0.031
122.	BD	(1)Sb	13-	O	22	551.	RY	(14)Sb	13			0.54	1.82	0.028
122.	BD	(1)Sb	13-	O	22	560.	RY	(23)Sb	13			0.86	2.58	0.042
122.	BD	(1)Sb	13-	O	22	794.	RY	(1) O	22			6.69	1.52	0.090
122.	BD	(1)Sb	13-	O	22	795.	RY	(2) O	22			9.85	1.71	0.116
122.	BD	(1)Sb	13-	O	22	796.	RY	(3) O	22			0.70	1.65	0.030
122.	BD	(1)Sb	13-	O	22	797.	RY	(4) O	22			1.18	2.50	0.049
122.	BD	(1)Sb	13-	O	22	819.	RY	(26) O	22			1.04	5.19	0.066
122.	BD	(1)Sb	13-	O	22	1028.	RY	(1) C	31			1.13	1.78	0.040
122.	BD	(1)Sb	13-	O	22	1029.	RY	(2) C	31			0.99	2.11	0.041
122.	BD	(1)Sb	13-	O	22	1030.	RY	(3) C	31			0.66	2.28	0.035
122.	BD	(1)Sb	13-	O	22	1042.	RY	(15) C	31			0.70	2.95	0.041
123.	BD	(1)Sb	14-	O	19	190.	BD*	(1)Sb	14-	O	19	13.94	0.80	0.094
123.	BD	(1)Sb	14-	O	19	191.	BD*	(1)Sb	14-	O	25	1.31	0.81	0.029
123.	BD	(1)Sb	14-	O	19	197.	BD*	(1) O	19-	C	29	0.52	0.84	0.019
123.	BD	(1)Sb	14-	O	19	210.	BD*	(1) C	28-	C	29	1.34	0.94	0.032
123.	BD	(1)Sb	14-	O	19	212.	BD*	(1) C	29-	C	30	1.30	0.92	0.031
123.	BD	(1)Sb	14-	O	19	213.	BD*	(1) C	29-	H	59	0.65	1.05	0.023
123.	BD	(1)Sb	14-	O	19	576.	RY	(2)Sb	14			0.65	2.32	0.035
123.	BD	(1)Sb	14-	O	19	595.	RY	(21)Sb	14			0.56	2.34	0.032
123.	BD	(1)Sb	14-	O	19	597.	RY	(23)Sb	14			0.53	2.53	0.033
123.	BD	(1)Sb	14-	O	19	716.	RY	(1) O	19			0.98	1.97	0.039
123.	BD	(1)Sb	14-	O	19	717.	RY	(2) O	19			1.59	1.92	0.049
123.	BD	(1)Sb	14-	O	19	718.	RY	(3) O	19			3.86	2.07	0.080
123.	BD	(1)Sb	14-	O	19	719.	RY	(4) O	19			0.61	2.15	0.032
123.	BD	(1)Sb	14-	O	19	727.	RY	(12) O	19			0.67	5.09	0.052
123.	BD	(1)Sb	14-	O	19	976.	RY	(1) C	29			3.34	1.98	0.073
124.	BD	(1)Sb	14-	O	25	190.	BD*	(1)Sb	14-	O	19	1.49	0.83	0.031
124.	BD	(1)Sb	14-	O	25	191.	BD*	(1)Sb	14-	O	25	13.72	0.84	0.096
124.	BD	(1)Sb	14-	O	25	205.	BD*	(1) O	25-	C	33	0.54	0.84	0.019
124.	BD	(1)Sb	14-	O	25	217.	BD*	(1) C	32-	C	33	1.89	0.94	0.038
124.	BD	(1)Sb	14-	O	25	219.	BD*	(1) C	33-	C	34	0.97	0.95	0.027
124.	BD	(1)Sb	14-	O	25	717.	RY	(2) O	19			0.51	1.95	0.028
124.	BD	(1)Sb	14-	O	25	872.	RY	(1) O	25			0.95	2.05	0.039
124.	BD	(1)Sb	14-	O	25	873.	RY	(2) O	25			1.36	1.91	0.045
124.	BD	(1)Sb	14-	O	25	874.	RY	(3) O	25			3.74	2.21	0.081
124.	BD	(1)Sb	14-	O	25	879.	RY	(8) O	25			0.58	3.48	0.040
124.	BD	(1)Sb	14-	O	25	883.	RY	(12) O	25			0.58	5.08	0.049
124.	BD	(1)Sb	14-	O	25	1080.	RY	(1) C	33			1.46	1.78	0.046
124.	BD	(1)Sb	14-	O	25	1082.	RY	(3) C	33			1.21	2.15	0.046
124.	BD	(1)Sb	14-	O	25	1262.	RY	(1) H	61			0.75	2.29	0.037
125.	BD	(1) O	15-	C	27	189.	BD*	(1)Sb	13-	O	22	1.72	1.15	0.040
125.	BD	(1) O	15-	C	27	192.	BD*	(1) O	15-	C	27	6.18	1.38	0.082
125.	BD	(1) O	15-	C	27	194.	BD*	(1) O	17-	C	27	0.74	1.38	0.028
125.	BD	(1) O	15-	C	27	195.	BD*	(1) O	17-	H	53	0.79	1.37	0.029
125.	BD	(1) O	15-	C	27	628.	RY	(17) O	15			0.50	23.26	0.096
125.	BD	(1) O	15-	C	27	924.	RY	(1) C	27			1.99	2.29	0.060
125.	BD	(1) O	15-	C	27	925.	RY	(2) C	27			2.29	2.66	0.070
126.	BD	(1) O	16-	C	28	193.	BD*	(1) O	16-	C	28	9.80	0.99	0.088
126.	BD	(1) O	16-	C	28	194.	BD*	(1) O	17-	C	27	1.18	1.20	0.034
126.	BD	(1) O	16-	C	28	213.	BD*	(1) C	29-	H	59	0.62	1.25	0.025
126.	BD	(1) O	16-	C	28	546.	RY	(9)Sb	13			0.59	2.27	0.033
126.	BD	(1) O	16-	C	28	547.	RY	(10)Sb	13			0.53	2.06	0.029
126.	BD	(1) O	16-	C	28	639.	RY	(2) O	16			0.58	1.98	0.030
126.	BD	(1) O	16-	C	28	641.	RY	(4) O	16			0.74	2.47	0.038
126.	BD	(1) O	16-	C	28	951.	RY	(2) C	28			2.39	2.11	0.063
126.	BD	(1) O	16-	C	28	952.	RY	(3) C	28			1.29	2.26	0.048
126.	BD	(1) O	16-	C	28	957.	RY	(8) C	28			0.69	3.10	0.041
126.	BD	(1) O	16-	C	28	960.	RY	(11) C	28			0.61	3.70	0.043
127.	BD	(1) O	17-	C	27	192.	BD*	(1) O	15-	C	27	0.72	1.45	0.029
127.	BD	(1) O	17-	C	27	194.	BD*	(1) O	17-	C	27	6.66	1.46	0.088
127.	BD	(1) O	17-	C	27	666.	RY	(3) O	17			0.51	3.33	0.037
127.	BD	(1) O	17-	C	27	680.	RY	(17) O	17			0.71	5.22	0.054
127.	BD	(1) O	17-	C	27	683.	RY	(20) O	17			0.51	15.74	0.080
127.	BD	(1) O	17-	C	27	688.	RY	(25) O	17			0.60	10.51	0.071
127.	BD	(1) O	17-	C	27	924.	RY	(1) C	27			1.66	2.37	0.056
127.	BD	(1) O	17-	C	27	925.	RY	(2) C	27			0.91	2.74	0.045
127.	BD	(1) O	17-	C	27	929.	RY	(6) C	27			0.66	4.17	0.047
128.	BD	(1) O	17-	H	53	192.	BD*	(1) O	15-	C	27	8.30	1.17	0.088
128.	BD	(1) O	17-	H	53	195.	BD*	(1) O	17-	H	53	20.55	1.17	0.138
128.	BD	(1) O	17-	H	53	208.	BD*	(1) C	27-	C	28	0.58	1.10	0.022
128.	BD	(1) O	17-	H	53	665.	RY	(2) O	17			1.03	2.04	0.041

128. BD (1) O 17- H 53	671. RY (8) O 17	3.08	3.46	0.092
128. BD (1) O 17- H 53	924. RY (1) C 27	3.83	2.09	0.080
128. BD (1) O 17- H 53	930. RY (7) C 27	0.72	3.94	0.047
128. BD (1) O 17- H 53	1222. RY (1) H 53	1.39	1.97	0.047
128. BD (1) O 17- H 53	1225. RY (4) H 53	1.27	3.12	0.056
129. BD (1) O 18- C 30	156. LV (1) Sb 14	1.93	1.04	0.040
129. BD (1) O 18- C 30	196. BD* (1) O 18- C 30	6.11	1.21	0.077
129. BD (1) O 18- C 30	198. BD* (1) O 20- C 30	0.51	1.33	0.023
129. BD (1) O 18- C 30	199. BD* (1) O 20- H 54	1.04	1.28	0.033
129. BD (1) O 18- C 30	578. RY (4) Sb 14	0.66	1.96	0.032
129. BD (1) O 18- C 30	1002. RY (1) C 30	0.76	2.26	0.037
129. BD (1) O 18- C 30	1003. RY (2) C 30	3.54	2.56	0.085
130. BD (1) O 19- C 29	197. BD* (1) O 19- C 29	9.34	1.08	0.090
130. BD (1) O 19- C 29	198. BD* (1) O 20- C 30	1.01	1.27	0.032
130. BD (1) O 19- C 29	578. RY (4) Sb 14	0.58	1.91	0.030
130. BD (1) O 19- C 29	583. RY (9) Sb 14	1.11	2.35	0.046
130. BD (1) O 19- C 29	719. RY (4) O 19	0.88	2.39	0.041
130. BD (1) O 19- C 29	846. RY (1) O 24	0.50	1.96	0.028
130. BD (1) O 19- C 29	976. RY (1) C 29	3.52	2.22	0.079
130. BD (1) O 19- C 29	978. RY (3) C 29	0.53	2.38	0.032
131. BD (1) O 20- C 30	196. BD* (1) O 18- C 30	0.59	1.41	0.026
131. BD (1) O 20- C 30	198. BD* (1) O 20- C 30	7.04	1.52	0.092
131. BD (1) O 20- C 30	744. RY (3) O 20	0.51	2.97	0.035
131. BD (1) O 20- C 30	766. RY (25) O 20	0.59	14.45	0.083
131. BD (1) O 20- C 30	1002. RY (1) C 30	2.24	2.46	0.066
131. BD (1) O 20- C 30	1013. RY (12) C 30	0.65	3.00	0.039
132. BD (1) O 20- H 54	196. BD* (1) O 18- C 30	9.33	1.11	0.091
132. BD (1) O 20- H 54	199. BD* (1) O 20- H 54	20.40	1.17	0.138
132. BD (1) O 20- H 54	212. BD* (1) C 29- C 30	0.72	1.10	0.025
132. BD (1) O 20- H 54	743. RY (2) O 20	1.18	2.07	0.044
132. BD (1) O 20- H 54	748. RY (7) O 20	0.73	3.97	0.048
132. BD (1) O 20- H 54	750. RY (9) O 20	2.06	3.42	0.075
132. BD (1) O 20- H 54	1002. RY (1) C 30	4.58	2.15	0.089
132. BD (1) O 20- H 54	1005. RY (4) C 30	0.88	3.10	0.047
132. BD (1) O 20- H 54	1007. RY (6) C 30	0.66	3.89	0.045
132. BD (1) O 20- H 54	1227. RY (1) H 54	0.79	1.88	0.034
132. BD (1) O 20- H 54	1229. RY (3) H 54	0.55	3.02	0.036
132. BD (1) O 20- H 54	1230. RY (4) H 54	1.17	3.09	0.054
133. BD (1) O 21- C 32	200. BD* (1) O 21- C 32	10.27	0.97	0.089
133. BD (1) O 21- C 32	202. BD* (1) O 23- C 31	1.43	1.21	0.037
133. BD (1) O 21- C 32	220. BD* (1) C 33- H 63	0.51	1.24	0.022
133. BD (1) O 21- C 32	541. RY (4) Sb 13	0.55	1.90	0.029
133. BD (1) O 21- C 32	546. RY (9) Sb 13	0.79	2.25	0.038
133. BD (1) O 21- C 32	612. RY (1) O 15	0.52	1.89	0.028
133. BD (1) O 21- C 32	769. RY (2) O 21	0.58	2.02	0.031
133. BD (1) O 21- C 32	771. RY (4) O 21	1.29	2.24	0.048
133. BD (1) O 21- C 32	1054. RY (1) C 32	2.60	2.09	0.066
133. BD (1) O 21- C 32	1055. RY (2) C 32	1.02	2.17	0.042
133. BD (1) O 21- C 32	1056. RY (3) C 32	0.53	2.30	0.031
133. BD (1) O 21- C 32	1058. RY (5) C 32	0.58	2.63	0.035
134. BD (1) O 22- C 31	189. BD* (1) Sb 13- O 22	0.79	1.11	0.027
134. BD (1) O 22- C 31	201. BD* (1) O 22- C 31	7.34	1.29	0.087
134. BD (1) O 22- C 31	203. BD* (1) O 23- H 55	0.99	1.33	0.032
134. BD (1) O 22- C 31	1028. RY (1) C 31	1.12	2.29	0.045
134. BD (1) O 22- C 31	1029. RY (2) C 31	3.22	2.62	0.082
135. BD (1) O 23- C 31	201. BD* (1) O 22- C 31	0.88	1.44	0.032
135. BD (1) O 23- C 31	202. BD* (1) O 23- C 31	6.83	1.52	0.091
135. BD (1) O 23- C 31	838. RY (19) O 23	0.65	20.21	0.103
135. BD (1) O 23- C 31	843. RY (24) O 23	0.62	14.95	0.086
135. BD (1) O 23- C 31	1028. RY (1) C 31	2.05	2.44	0.063
135. BD (1) O 23- C 31	1032. RY (5) C 31	0.52	3.95	0.041
135. BD (1) O 23- C 31	1042. RY (15) C 31	0.51	3.62	0.038
136. BD (1) O 23- H 55	201. BD* (1) O 22- C 31	9.36	1.13	0.092
136. BD (1) O 23- H 55	203. BD* (1) O 23- H 55	20.49	1.17	0.138
136. BD (1) O 23- H 55	215. BD* (1) C 31- C 32	0.61	1.12	0.023
136. BD (1) O 23- H 55	821. RY (2) O 23	1.19	2.06	0.044
136. BD (1) O 23- H 55	823. RY (4) O 23	0.53	2.84	0.035
136. BD (1) O 23- H 55	825. RY (6) O 23	0.94	2.87	0.046
136. BD (1) O 23- H 55	828. RY (9) O 23	1.07	3.95	0.058
136. BD (1) O 23- H 55	1028. RY (1) C 31	4.72	2.14	0.090
136. BD (1) O 23- H 55	1033. RY (6) C 31	0.62	3.87	0.044
136. BD (1) O 23- H 55	1232. RY (1) H 55	0.69	2.00	0.033
136. BD (1) O 23- H 55	1233. RY (2) H 55	0.60	2.98	0.038
136. BD (1) O 23- H 55	1234. RY (3) H 55	0.52	3.04	0.036
136. BD (1) O 23- H 55	1235. RY (4) H 55	1.06	3.03	0.051
137. BD (1) O 24- C 34	156. LV (1) Sb 14	2.16	1.09	0.043
137. BD (1) O 24- C 34	204. BD* (1) O 24- C 34	6.16	1.31	0.080
137. BD (1) O 24- C 34	206. BD* (1) O 26- C 34	0.62	1.36	0.026
137. BD (1) O 24- C 34	207. BD* (1) O 26- H 56	0.96	1.33	0.032
137. BD (1) O 24- C 34	578. RY (4) Sb 14	0.69	2.01	0.033
137. BD (1) O 24- C 34	1106. RY (1) C 34	1.22	2.28	0.047
137. BD (1) O 24- C 34	1107. RY (2) C 34	2.61	2.61	0.074
137. BD (1) O 24- C 34	1109. RY (4) C 34	0.54	2.31	0.031
137. BD (1) O 24- C 34	1118. RY (13) C 34	0.57	3.62	0.041
138. BD (1) O 25- C 33	205. BD* (1) O 25- C 33	9.28	1.05	0.088
138. BD (1) O 25- C 33	206. BD* (1) O 26- C 34	1.15	1.26	0.034
138. BD (1) O 25- C 33	584. RY (10) Sb 14	0.99	2.27	0.042
138. BD (1) O 25- C 33	875. RY (4) O 25	0.58	2.57	0.034
138. BD (1) O 25- C 33	1080. RY (1) C 33	0.69	1.99	0.033
138. BD (1) O 25- C 33	1081. RY (2) C 33	0.90	2.15	0.039
138. BD (1) O 25- C 33	1082. RY (3) C 33	2.32	2.36	0.066
138. BD (1) O 25- C 33	1087. RY (8) C 33	0.83	3.44	0.048
138. BD (1) O 25- C 33	1090. RY (11) C 33	0.64	3.74	0.044
139. BD (1) O 26- C 34	204. BD* (1) O 24- C 34	0.61	1.45	0.026
139. BD (1) O 26- C 34	206. BD* (1) O 26- C 34	6.74	1.49	0.090
139. BD (1) O 26- C 34	904. RY (7) O 26	0.52	4.08	0.041
139. BD (1) O 26- C 34	910. RY (13) O 26	0.52	4.77	0.044
139. BD (1) O 26- C 34	918. RY (21) O 26	0.62	16.41	0.090
139. BD (1) O 26- C 34	922. RY (25) O 26	0.50	10.39	0.064
139. BD (1) O 26- C 34	1106. RY (1) C 34	2.03	2.41	0.062
139. BD (1) O 26- C 34	1107. RY (2) C 34	0.55	2.74	0.035
139. BD (1) O 26- C 34	1111. RY (6) C 34	0.61	4.18	0.045
139. BD (1) O 26- C 34	1118. RY (13) C 34	0.69	3.76	0.045

140.	BD	(1)	O 26-	H 56	204.	BD*	(1)	O 24-	C 34	8.96	1.15	0.090
140.	BD	(1)	O 26-	H 56	207.	BD*	(1)	O 26-	H 56	20.65	1.16	0.138
140.	BD	(1)	O 26-	H 56	219.	BD*	(1)	C 33-	C 34	0.59	1.10	0.023
140.	BD	(1)	O 26-	H 56	899.	RY	(2)	O 26		1.04	2.05	0.041
140.	BD	(1)	O 26-	H 56	903.	RY	(6)	O 26		0.63	2.62	0.036
140.	BD	(1)	O 26-	H 56	905.	RY	(8)	O 26		0.73	4.51	0.051
140.	BD	(1)	O 26-	H 56	906.	RY	(9)	O 26		1.93	3.82	0.077
140.	BD	(1)	O 26-	H 56	1106.	RY	(1)	C 34		4.60	2.11	0.088
140.	BD	(1)	O 26-	H 56	1112.	RY	(7)	C 34		0.83	3.95	0.051
140.	BD	(1)	O 26-	H 56	1237.	RY	(1)	H 56		1.25	1.91	0.044
140.	BD	(1)	O 26-	H 56	1239.	RY	(3)	H 56		0.54	3.02	0.036
140.	BD	(1)	O 26-	H 56	1240.	RY	(4)	H 56		1.21	3.14	0.055
141.	BD	(1)	C 27-	C 28	193.	BD*	(1)	O 16-	C 28	0.61	0.75	0.019
141.	BD	(1)	C 27-	C 28	212.	BD*	(1)	C 29-	C 30	1.83	0.87	0.036
141.	BD	(1)	C 27-	C 28	665.	RY	(2)	O 17		0.86	1.83	0.035
141.	BD	(1)	C 27-	C 28	928.	RY	(5)	C 27		0.72	2.86	0.041
141.	BD	(1)	C 27-	C 28	938.	RY	(15)	C 27		0.61	3.09	0.039
141.	BD	(1)	C 27-	C 28	953.	RY	(4)	C 28		0.99	2.13	0.041
141.	BD	(1)	C 27-	C 28	957.	RY	(8)	C 28		0.87	2.86	0.044
142.	BD	(1)	C 27-	H 57	209.	BD*	(1)	C 27-	H 57	10.50	0.77	0.080
142.	BD	(1)	C 27-	H 57	210.	BD*	(1)	C 28-	C 29	4.78	0.71	0.052
142.	BD	(1)	C 27-	H 57	211.	BD*	(1)	C 28-	H 58	1.01	0.83	0.026
142.	BD	(1)	C 27-	H 57	612.	RY	(1)	O 15		1.44	1.49	0.041
142.	BD	(1)	C 27-	H 57	664.	RY	(1)	O 17		2.36	1.48	0.053
142.	BD	(1)	C 27-	H 57	927.	RY	(4)	C 27		1.27	1.79	0.043
142.	BD	(1)	C 27-	H 57	931.	RY	(8)	C 27		0.59	2.60	0.035
142.	BD	(1)	C 27-	H 57	1242.	RY	(1)	H 57		2.27	1.58	0.054
142.	BD	(1)	C 27-	H 57	1245.	RY	(4)	H 57		1.38	2.81	0.056
143.	BD	(1)	C 28-	C 29	187.	BD*	(1)	Sb 13-	O 16	0.53	0.76	0.018
143.	BD	(1)	C 28-	C 29	190.	BD*	(1)	Sb 14-	O 19	0.51	0.77	0.018
143.	BD	(1)	C 28-	C 29	192.	BD*	(1)	O 15-	C 27	0.66	0.97	0.023
143.	BD	(1)	C 28-	C 29	196.	BD*	(1)	O 18-	C 30	1.22	0.89	0.029
143.	BD	(1)	C 28-	C 29	950.	RY	(1)	C 28		0.92	1.68	0.035
143.	BD	(1)	C 28-	C 29	979.	RY	(4)	C 29		0.82	2.20	0.038
143.	BD	(1)	C 28-	C 29	997.	RY	(22)	C 29		0.65	9.82	0.072
144.	BD	(1)	C 28-	H 58	192.	BD*	(1)	O 15-	C 27	1.28	0.86	0.030
144.	BD	(1)	C 28-	H 58	193.	BD*	(1)	O 16-	C 28	1.29	0.65	0.026
144.	BD	(1)	C 28-	H 58	197.	BD*	(1)	O 19-	C 29	3.62	0.70	0.045
144.	BD	(1)	C 28-	H 58	211.	BD*	(1)	C 28-	H 58	5.30	0.92	0.062
144.	BD	(1)	C 28-	H 58	951.	RY	(2)	C 28		0.58	1.77	0.029
144.	BD	(1)	C 28-	H 58	952.	RY	(3)	C 28		1.74	1.92	0.052
144.	BD	(1)	C 28-	H 58	956.	RY	(7)	C 28		0.63	2.46	0.035
144.	BD	(1)	C 28-	H 58	961.	RY	(12)	C 28		0.70	4.47	0.050
144.	BD	(1)	C 28-	H 58	979.	RY	(4)	C 29		0.67	2.10	0.034
144.	BD	(1)	C 28-	H 58	1247.	RY	(1)	H 58		1.84	1.74	0.050
144.	BD	(1)	C 28-	H 58	1250.	RY	(4)	H 58		0.97	3.11	0.049
145.	BD	(1)	C 29-	C 30	197.	BD*	(1)	O 19-	C 29	0.58	0.79	0.019
145.	BD	(1)	C 29-	C 30	208.	BD*	(1)	C 27-	C 28	1.23	0.87	0.029
145.	BD	(1)	C 29-	C 30	718.	RY	(3)	O 19		0.58	2.01	0.030
145.	BD	(1)	C 29-	C 30	743.	RY	(2)	O 20		0.54	1.83	0.028
145.	BD	(1)	C 29-	C 30	953.	RY	(4)	C 28		0.56	2.11	0.031
145.	BD	(1)	C 29-	C 30	978.	RY	(3)	C 29		0.77	2.09	0.036
145.	BD	(1)	C 29-	C 30	984.	RY	(9)	C 29		0.70	3.13	0.042
145.	BD	(1)	C 29-	C 30	1008.	RY	(7)	C 30		0.65	2.67	0.037
145.	BD	(1)	C 29-	C 30	1013.	RY	(12)	C 30		0.52	2.45	0.032
145.	BD	(1)	C 29-	C 30	1018.	RY	(17)	C 30		0.60	2.58	0.035
146.	BD	(1)	C 29-	H 59	190.	BD*	(1)	Sb 14-	O 19	0.86	0.64	0.021
146.	BD	(1)	C 29-	H 59	193.	BD*	(1)	O 16-	C 28	4.29	0.64	0.047
146.	BD	(1)	C 29-	H 59	196.	BD*	(1)	O 18-	C 30	0.63	0.77	0.020
146.	BD	(1)	C 29-	H 59	197.	BD*	(1)	O 19-	C 29	0.86	0.69	0.022
146.	BD	(1)	C 29-	H 59	212.	BD*	(1)	C 29-	C 30	0.55	0.76	0.018
146.	BD	(1)	C 29-	H 59	213.	BD*	(1)	C 29-	H 59	6.17	0.90	0.066
146.	BD	(1)	C 29-	H 59	214.	BD*	(1)	C 30-	H 60	0.60	0.87	0.020
146.	BD	(1)	C 29-	H 59	977.	RY	(2)	C 29		1.31	1.81	0.043
146.	BD	(1)	C 29-	H 59	979.	RY	(4)	C 29		0.58	2.08	0.031
146.	BD	(1)	C 29-	H 59	982.	RY	(7)	C 29		0.81	2.34	0.039
146.	BD	(1)	C 29-	H 59	985.	RY	(10)	C 29		0.86	4.20	0.054
146.	BD	(1)	C 29-	H 59	997.	RY	(22)	C 29		0.54	9.70	0.065
146.	BD	(1)	C 29-	H 59	1252.	RY	(1)	H 59		2.46	1.41	0.053
146.	BD	(1)	C 29-	H 59	1255.	RY	(4)	H 59		1.00	3.10	0.050
147.	BD	(1)	C 30-	H 60	208.	BD*	(1)	C 27-	C 28	0.90	0.71	0.023
147.	BD	(1)	C 30-	H 60	210.	BD*	(1)	C 28-	C 29	0.89	0.73	0.023
147.	BD	(1)	C 30-	H 60	213.	BD*	(1)	C 29-	H 59	3.72	0.84	0.050
147.	BD	(1)	C 30-	H 60	214.	BD*	(1)	C 30-	H 60	6.18	0.82	0.063
147.	BD	(1)	C 30-	H 60	690.	RY	(1)	O 18		1.22	1.52	0.038
147.	BD	(1)	C 30-	H 60	742.	RY	(1)	O 20		2.58	1.50	0.056
147.	BD	(1)	C 30-	H 60	1011.	RY	(10)	C 30		0.51	2.40	0.031
147.	BD	(1)	C 30-	H 60	1257.	RY	(1)	H 60		1.93	2.15	0.057
147.	BD	(1)	C 30-	H 60	1259.	RY	(3)	H 60		0.52	2.59	0.033
147.	BD	(1)	C 30-	H 60	1260.	RY	(4)	H 60		0.52	2.79	0.034
148.	BD	(1)	C 31-	C 32	200.	BD*	(1)	O 21-	C 32	0.73	0.75	0.021
148.	BD	(1)	C 31-	C 32	219.	BD*	(1)	C 33-	C 34	0.93	0.89	0.026
148.	BD	(1)	C 31-	C 32	821.	RY	(2)	O 23		0.53	1.84	0.028
148.	BD	(1)	C 31-	C 32	1031.	RY	(4)	C 31		0.51	2.73	0.033
148.	BD	(1)	C 31-	C 32	1043.	RY	(16)	C 31		0.58	2.96	0.037
148.	BD	(1)	C 31-	C 32	1044.	RY	(17)	C 31		0.69	2.52	0.037
148.	BD	(1)	C 31-	C 32	1056.	RY	(3)	C 32		0.51	2.09	0.029
148.	BD	(1)	C 31-	C 32	1061.	RY	(8)	C 32		0.67	2.47	0.036
148.	BD	(1)	C 31-	C 32	1083.	RY	(4)	C 33		0.58	2.16	0.031
149.	BD	(1)	C 31-	H 61	189.	BD*	(1)	Sb 13-	O 22	1.76	0.57	0.028
149.	BD	(1)	C 31-	H 61	216.	BD*	(1)	C 31-	H 61	5.98	0.82	0.062
149.	BD	(1)	C 31-	H 61	217.	BD*	(1)	C 32-	C 33	1.15	0.71	0.026
149.	BD	(1)	C 31-	H 61	218.	BD*	(1)	C 32-	H 62	4.27	0.85	0.054
149.	BD	(1)	C 31-	H 61	219.	BD*	(1)	C 33-	C 34	0.68	0.72	0.020
149.	BD	(1)	C 31-	H 61	794.	RY	(1)	O 22		1.42	1.50	0.041
149.	BD	(1)	C 31-	H 61	820.	RY	(1)	O 23		2.54	1.47	0.054
149.	BD	(1)	C 31-	H 61	1038.	RY	(11)	C 31		0.57	2.81	0.036
149.	BD	(1)	C 31-	H 61	1262.	RY	(1)	H 61		1.86	2.06	0.055
149.	BD	(1)	C 31-	H 61	1264.	RY	(3)	H 61		0.65	2.73	0.038
150.	BD	(1)	C 32-	C 33	191.	BD*	(1)	Sb 14-	O 25	0.75	0.76	0.021
150.	BD	(1)	C 32-	C 33	201.	BD*	(1)	O 22-	C 31	1.44	0.90	0.032
150.	BD	(1)	C 32-	C 33	204.	BD*	(1)	O 24-	C 34	0.74	0.93	0.023
150.	BD	(1)	C 32-	C 33	1057.	RY	(4)	C 32		0.58	2.24	0.032

150. BD (1) C 32- C 33	1076. RY (23) C 32	0.61	13.45	0.081
150. BD (1) C 32- C 33	1080. RY (1) C 33	0.58	1.71	0.028
150. BD (1) C 32- C 33	1083. RY (4) C 33	0.73	2.15	0.035
151. BD (1) C 32- H 62	188. BD* (1) Sb 13- O 21	0.54	0.64	0.017
151. BD (1) C 32- H 62	200. BD* (1) O 21- C 32	0.92	0.64	0.022
151. BD (1) C 32- H 62	201. BD* (1) O 22- C 31	0.54	0.80	0.019
151. BD (1) C 32- H 62	205. BD* (1) O 25- C 33	3.75	0.67	0.045
151. BD (1) C 32- H 62	215. BD* (1) C 31- C 32	0.56	0.79	0.019
151. BD (1) C 32- H 62	216. BD* (1) C 31- H 61	0.75	0.87	0.023
151. BD (1) C 32- H 62	217. BD* (1) C 32- C 33	0.52	0.77	0.018
151. BD (1) C 32- H 62	218. BD* (1) C 32- H 62	5.84	0.90	0.065
151. BD (1) C 32- H 62	1055. RY (2) C 32	0.82	1.84	0.035
151. BD (1) C 32- H 62	1057. RY (4) C 32	0.72	2.13	0.035
151. BD (1) C 32- H 62	1060. RY (7) C 32	0.85	2.43	0.041
151. BD (1) C 32- H 62	1063. RY (10) C 32	0.88	4.01	0.053
151. BD (1) C 32- H 62	1267. RY (1) H 62	2.40	1.39	0.052
151. BD (1) C 32- H 62	1270. RY (4) H 62	1.15	3.08	0.053
152. BD (1) C 33- C 34	215. BD* (1) C 31- C 32	1.68	0.90	0.035
152. BD (1) C 33- C 34	899. RY (2) O 26	0.85	1.84	0.035
152. BD (1) C 33- C 34	1083. RY (4) C 33	0.85	2.15	0.038
152. BD (1) C 33- C 34	1087. RY (8) C 33	0.57	3.16	0.038
152. BD (1) C 33- C 34	1110. RY (5) C 34	0.84	2.86	0.044
153. BD (1) C 33- H 63	191. BD* (1) Sb 14- O 25	0.55	0.67	0.017
153. BD (1) C 33- H 63	200. BD* (1) O 21- C 32	3.23	0.65	0.041
153. BD (1) C 33- H 63	204. BD* (1) O 24- C 34	1.11	0.84	0.027
153. BD (1) C 33- H 63	205. BD* (1) O 25- C 33	1.25	0.68	0.026
153. BD (1) C 33- H 63	220. BD* (1) C 33- H 63	5.41	0.92	0.063
153. BD (1) C 33- H 63	1057. RY (4) C 32	0.52	2.14	0.030
153. BD (1) C 33- H 63	1081. RY (2) C 33	1.07	1.77	0.039
153. BD (1) C 33- H 63	1082. RY (3) C 33	1.18	1.99	0.043
153. BD (1) C 33- H 63	1086. RY (7) C 33	0.92	2.61	0.044
153. BD (1) C 33- H 63	1091. RY (12) C 33	0.83	4.54	0.055
153. BD (1) C 33- H 63	1095. RY (16) C 33	0.51	5.72	0.048
153. BD (1) C 33- H 63	1101. RY (22) C 33	0.57	5.43	0.050
153. BD (1) C 33- H 63	1272. RY (1) H 63	1.80	1.78	0.050
153. BD (1) C 33- H 63	1275. RY (4) H 63	1.31	2.98	0.056
154. BD (1) C 34- H 64	217. BD* (1) C 32- C 33	4.50	0.69	0.050
154. BD (1) C 34- H 64	220. BD* (1) C 33- H 63	1.01	0.83	0.026
154. BD (1) C 34- H 64	221. BD* (1) C 34- H 64	10.12	0.78	0.079
154. BD (1) C 34- H 64	846. RY (1) O 24	1.27	1.49	0.039
154. BD (1) C 34- H 64	898. RY (1) O 26	2.35	1.46	0.052
154. BD (1) C 34- H 64	1109. RY (4) C 34	1.37	1.75	0.044
154. BD (1) C 34- H 64	1113. RY (8) C 34	0.54	2.67	0.034
154. BD (1) C 34- H 64	1277. RY (1) H 64	1.98	1.59	0.050
154. BD (1) C 34- H 64	1279. RY (3) H 64	1.33	2.82	0.055