

Mechanistic Studies for Dirhodium-Catalyzed Chemoselective Oxidative Amination of Alkynyl-tethered Sulfamates

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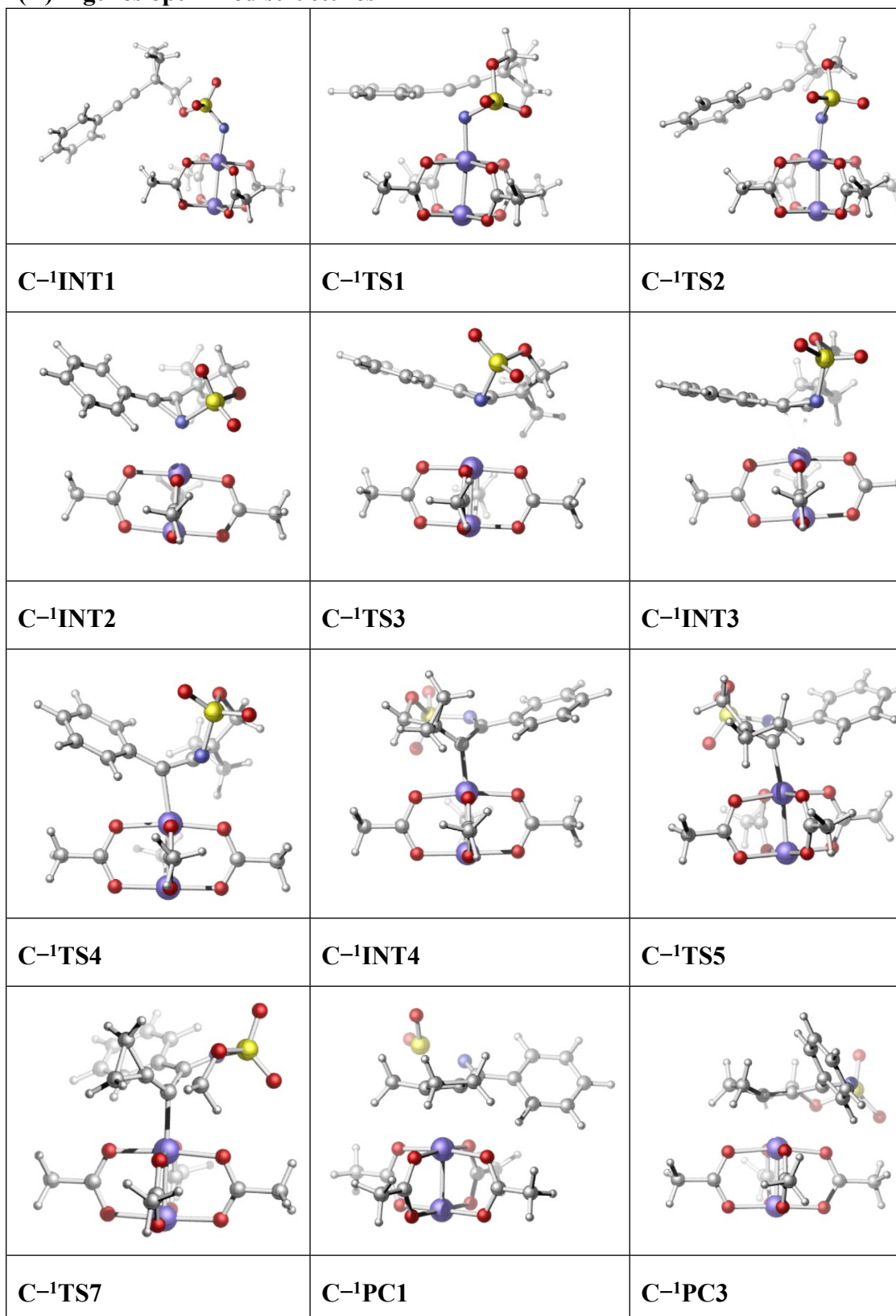
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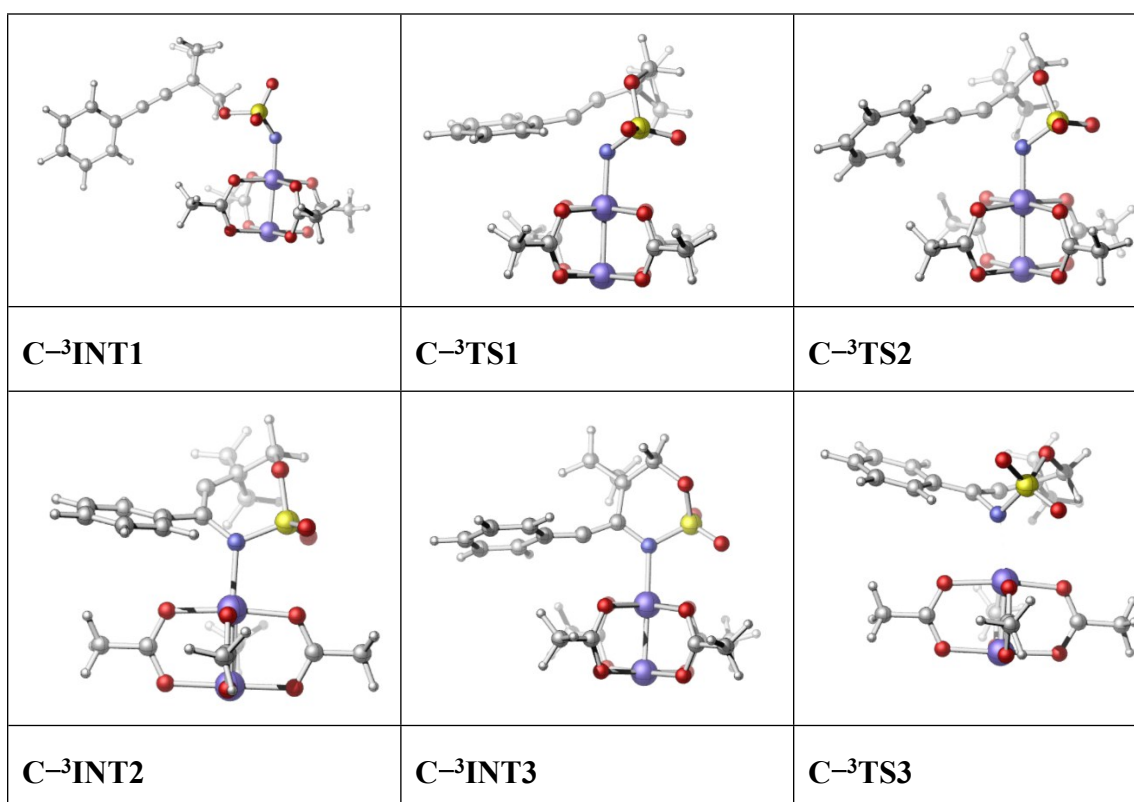
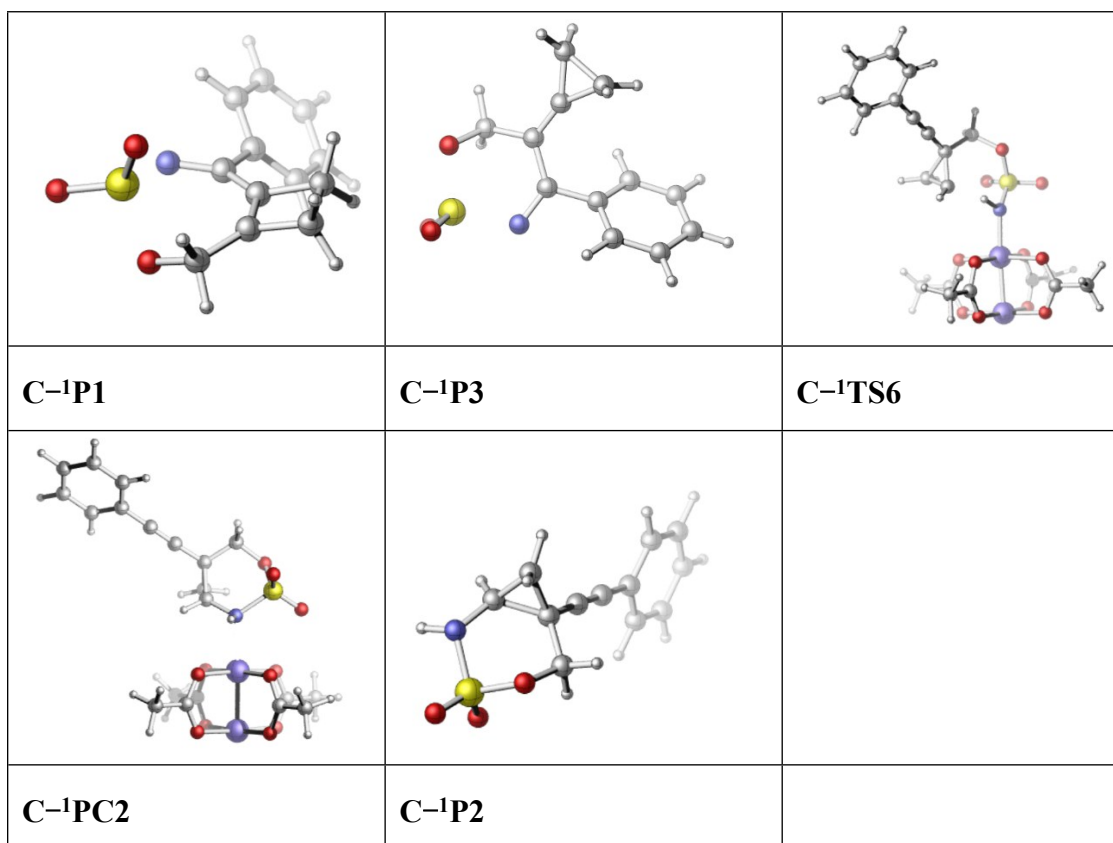
Supporting Information

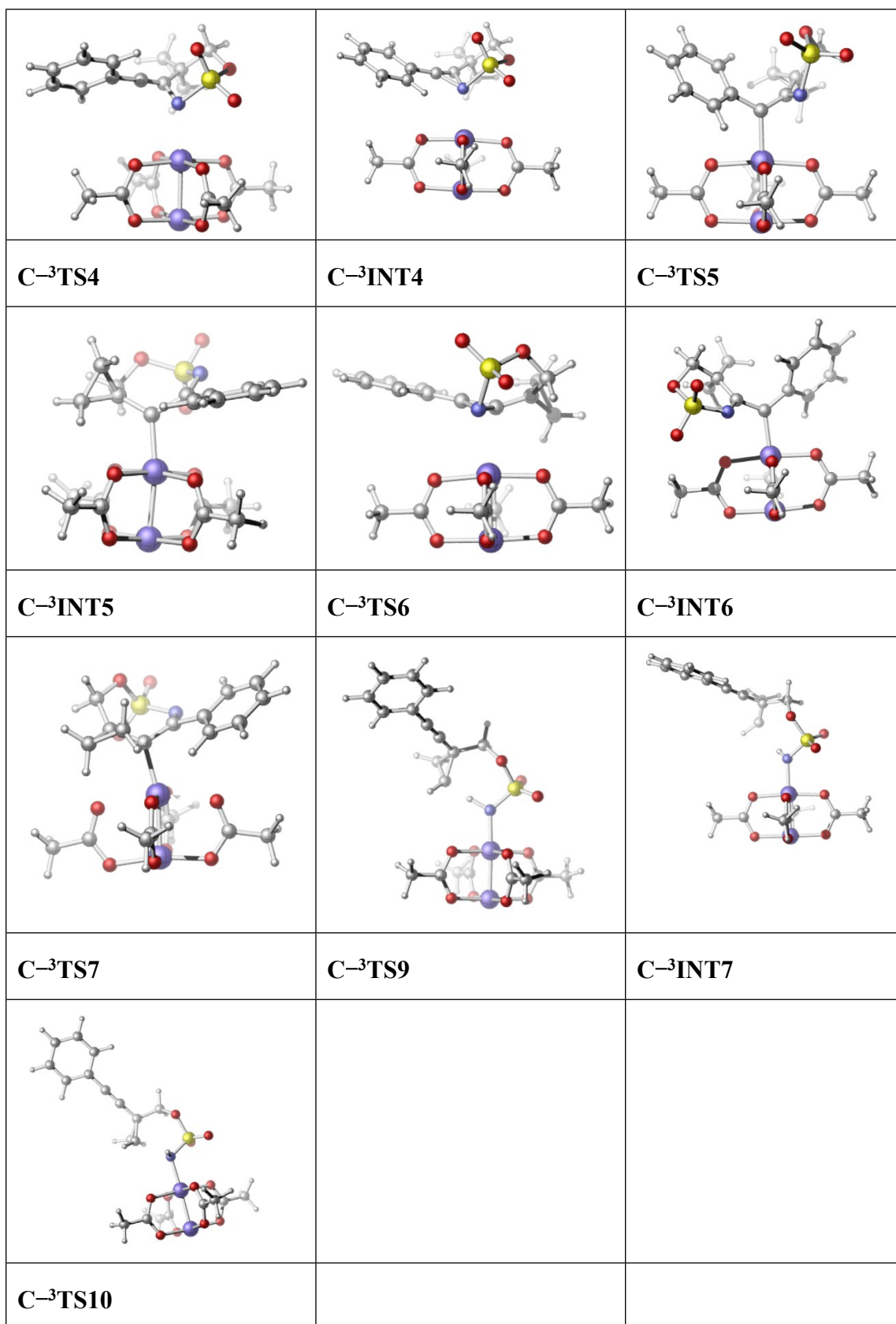
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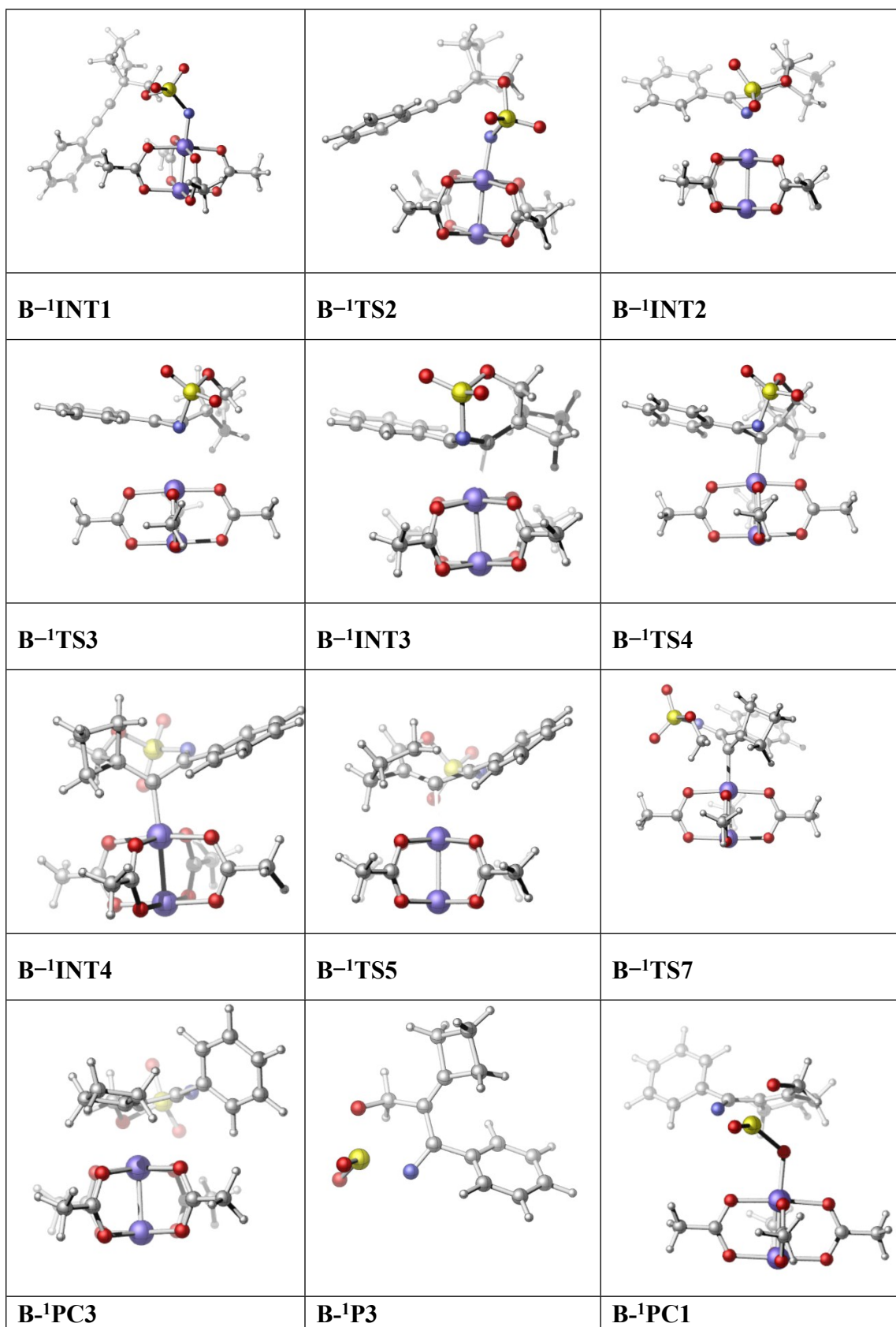
(A) Figures of the optimized structures.....	P2-P8
(B) The total energies, enthalpies and free energies of the lowest conformers of all species shown in Scheme 4-12.....	P8-P79

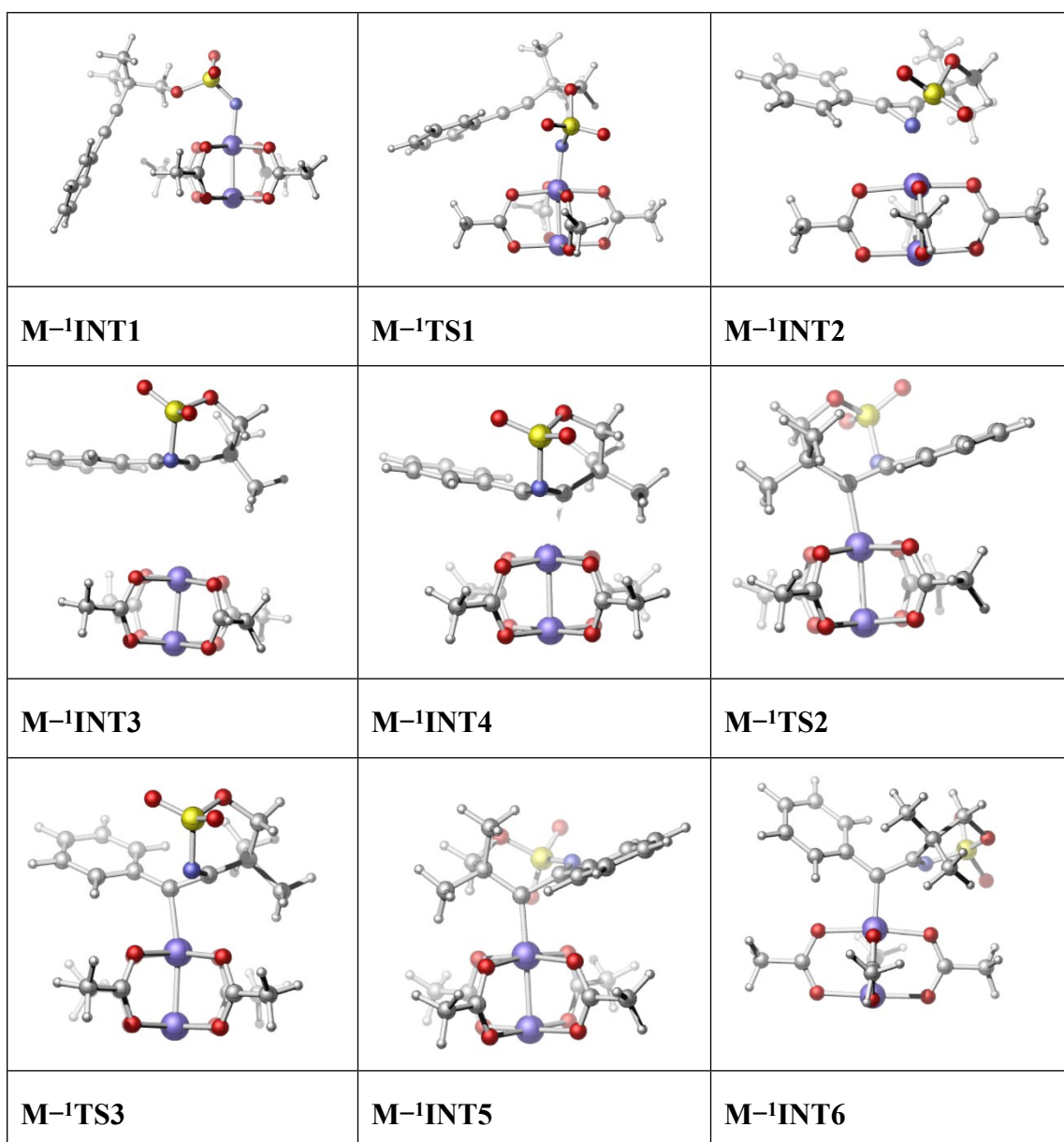
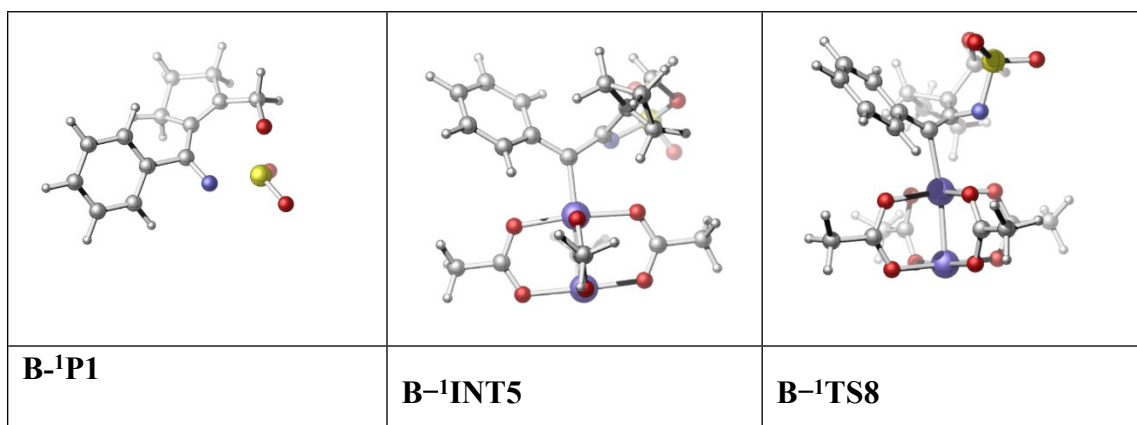
(A) Figures optimized structures

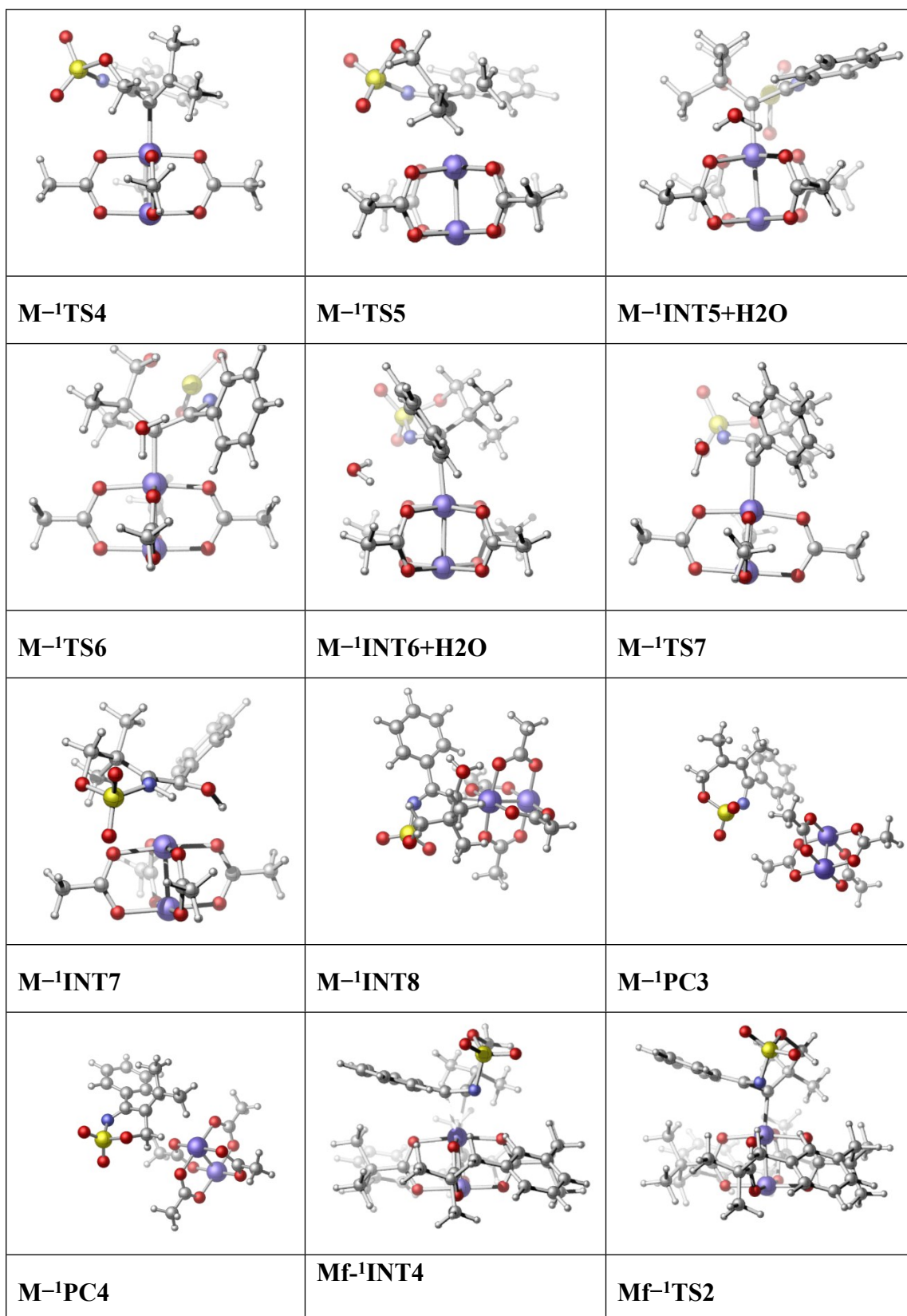


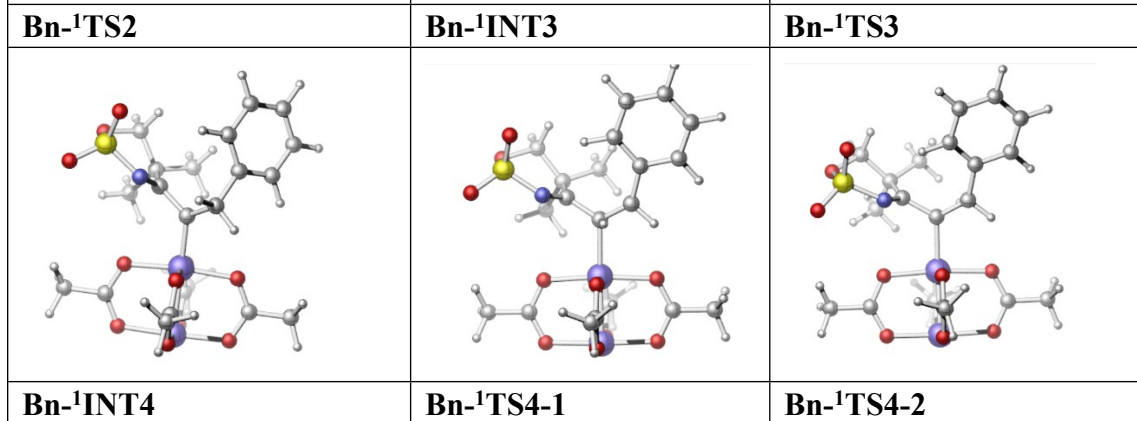
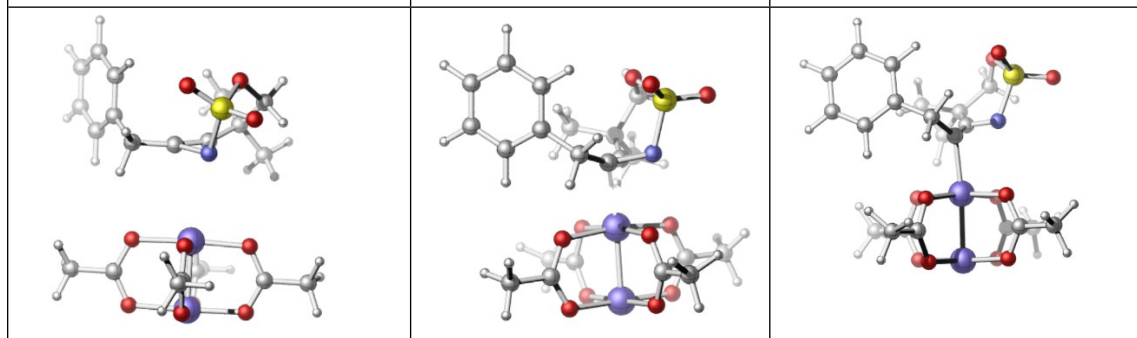
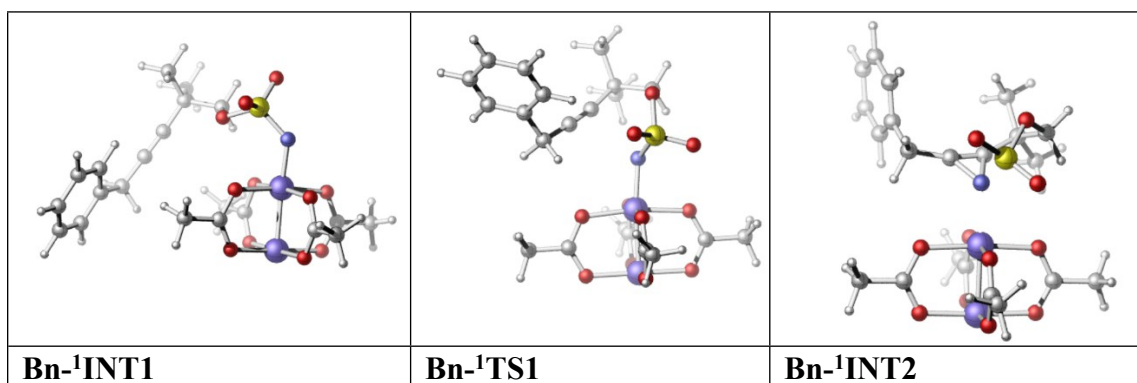
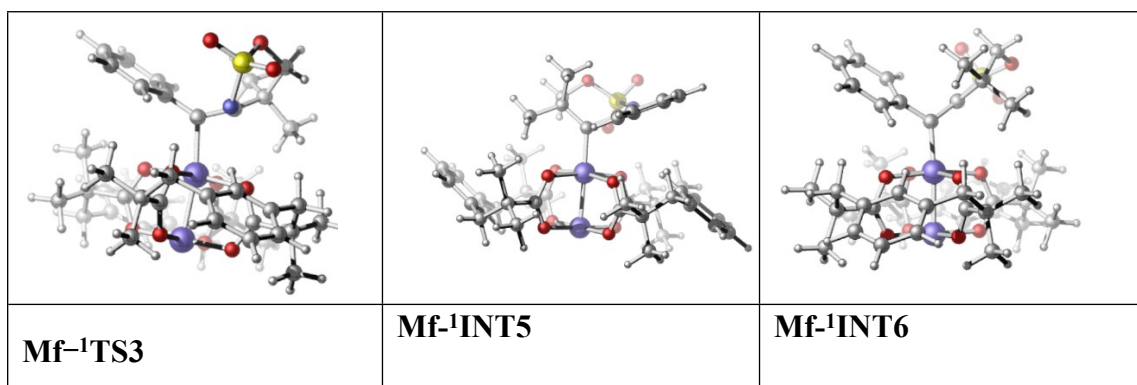


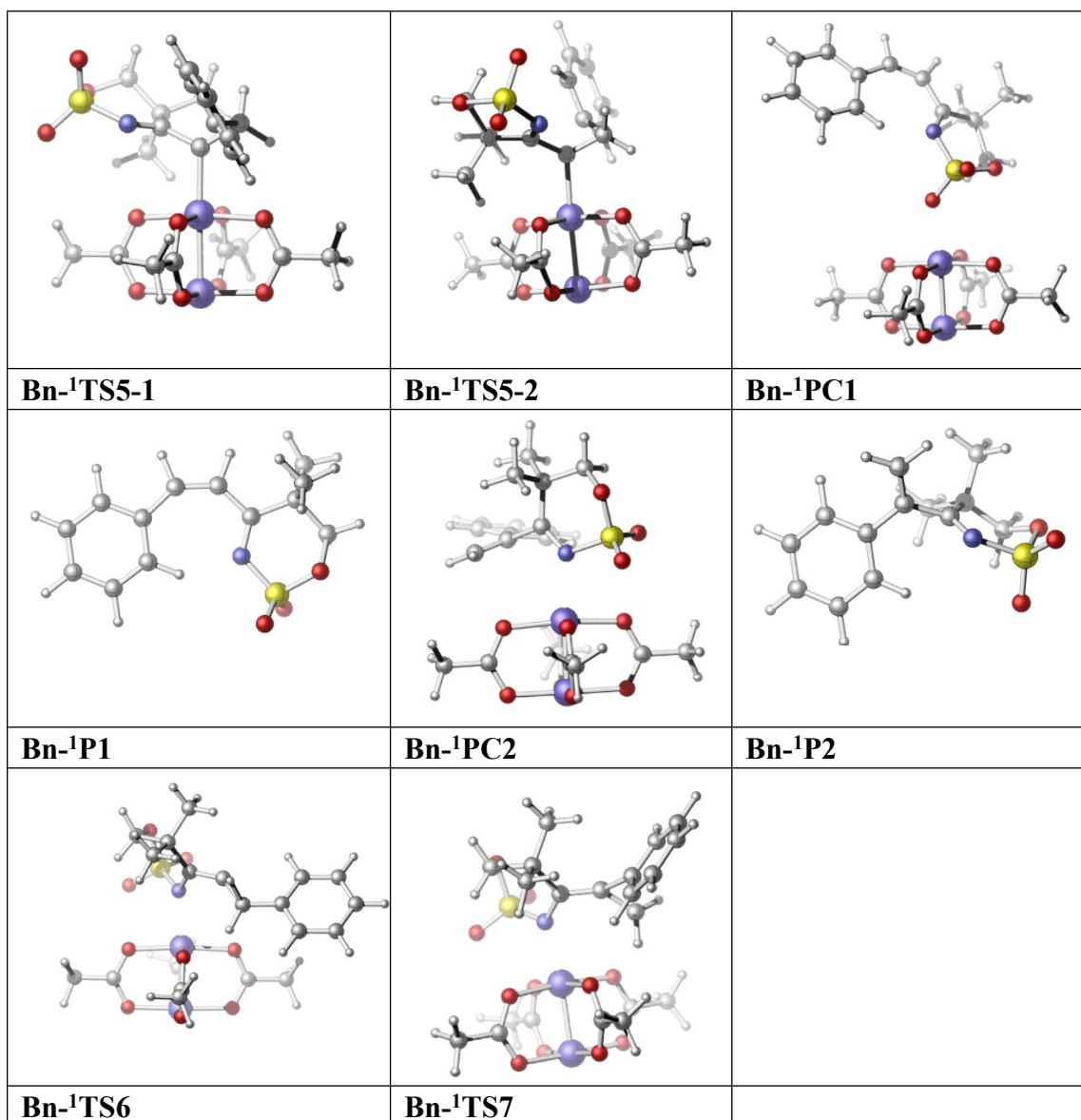












(B) The total energies, enthalpies and free energies of the lowest conformers of all species shown in Scheme 4-12 and optimized structures in Figures

The total energies, enthalpies and free energies of the lowest conformers of all species shown in Scheme 4 and archive entries^[1]

Table S1

	$E_{\text{tot}} (E_h)_{\text{DCM}}$	$G_{298, \text{DCM}}$	$H_{298, \text{DCM}}$	# of imaginary frequencies
C- ³ INT1	-2278.098384	-2277.539893	-2277.210078	0
C- ³ TS1	-2278.070140	-2277.517239	-2277.181806	1 (-336.5 cm-1)
C- ³ TS2	-2278.081567	-2277.526426	-2277.193461	1 (-295.1 cm-1)
C- ³ INT2	-2278.101866	-2277.553682	-2278.101866	0

C- ³ INT3	-2278.118620	-2277.569064	-2277.232475	0
C- ³ TS3	-2278.070694	-2277.518614	-2277.187383	1 (-583.8 cm-1)
C- ³ TS4	-2278.078722	-2277.528342	-2277.194040	1 (-316.5 cm-1)
C- ³ INT4	-2278.088876	-2277.537833	-2277.205665	0
C- ³ TS5	-2278.079242	-2277.527629	-2277.194802	1 (-204.7 cm-1)
C- ³ INT5	-2278.1180495	-2277.569130	-2277.230990	0
C- ³ TS6	-2278.082358	-2277.531743	-2277.199469	1 (-126.1 cm-1)
C- ³ INT6	-2278.129126	-2277.579942	-2277.240843	0
C- ³ TS7	-2278.084772	-2277.530848	-2277.195853	1 (-383.9 cm-1)
C- ¹ PC1	-2278.121082	-2277.075951	-2276.738043	0
C- ¹ P1	-1142.502880	-1142.313013	-1142.147836	0
Rh ₂ (OAc) ₄	-1135.633535	-1135.331132	-1135.177759	0
C- ³ TS9	-2278.070138	-2277.508570	-2277.182688	1 (-532.2 cm-1)
C- ³ INT7	-2278.074643	-2277.511659	-2277.182643	0
C- ³ TS10	-2278.061537	-2277.499466	-2277.172385	1 (-293.5 cm-1)
C- ¹ PC2	-2278.159086	-2277.603490	-2277.263959	0
C- ¹ P2	-1142.463577	-1142.267092	-1142.104812	0

The total energies, enthalpies and free energies of the lowest conformers of all species shown in Scheme 5 and Scheme 6 and archive entries

Table S2

	E _{tot} (E _h) _{DCM}	G _{298,DCM}	H _{298,DCM}	# of imaginary frequencies
C- ¹ INT1	-2278.094198	-2277.536388	-2277.205064	0
C- ¹ TS1	-2278.075558	-2277.523973	-2277.186989	1 (-181.0 cm-1)
C- ¹ TS2	-2278.084513	-2277.529476	-2277.194961	1 (-64.4 cm-1)
C- ¹ INT2	-2278.130171	-2277.579940	-2277.241487	0
C- ¹ TS3	-2278.113033	-2277.555833	-2277.221916	1 (-78.6 cm-1)
C- ¹ INT3	-2278.120142	-2277.572250	-2277.232489	0
C- ¹ TS4	-2278.117184	-2277.568783	-2277.228421	1 (-194.0 cm-1)
C- ¹ INT4	-2278.140489	-2277.595993	-2277.255380	0
C- ¹ TS5	-2278.123833	-2277.571361	-2277.230629	1 (-388.0 cm-1)
C- ¹ TS7	-2278.098216	-2277.548343	-2277.211210	1 (-333.9 cm-1)
C- ¹ PC1	-2278.121082	-2277.075951	-2276.738043	0
C- ¹ P1	-1142.502880	-1142.313013	-1142.147836	0
Rh ₂ (OAc) ₄	-1135.633535	-1135.331132	-1135.177759	0
C- ¹ TS6	-2278.067373	-2277.506526	-2277.177315	1 (-706.9 cm-1)
C- ¹ PC2	-2278.159086	-2277.603490	-2277.263959	0
C- ¹ P2	-1142.463577	-1142.267092	-1142.104812	0
C- ¹ PC3	-2278.105195	-2277.058451	-2276.719895	0
C- ¹ P3	-1142.487338	-1142.296709	-1142.133093	0

The total energies, enthalpies and free energies of the lowest conformers of all species shown in Scheme 7 and archive entries

Table S3

	$E_{\text{tot}} (E_h)_{\text{DCM}}$	$G_{298, \text{DCM}}$	$H_{298, \text{DCM}}$	# of imaginary frequencies
B- ¹ INT1	-2317.769543	-2316.843011	-2317.408963	0
B- ¹ TS2	-2317.402515	-2316.837165	-2316.473404	1 (-48.4 cm ⁻¹)
B- ¹ INT2	-2317.449557	-2316.889065	-2316.523102	0
B- ¹ TS3	-2317.430974	-2316.863987	-2316.502343	1 (-72.0 cm ⁻¹)
B- ¹ INT3	-2317.440065	-2316.881623	-2316.513896	0
B- ¹ TS4	-2317.435240	-2316.876749	-2316.509690	1 (-171.4 cm ⁻¹)
B- ¹ INT4	-2317.459774	-2316.905369	-2316.535247	0
B- ¹ TS5	-2317.429007	-2316.866313	-2316.499290	1 (-453.6 cm ⁻¹)
B- ¹ TS7	-2317.433832	-2316.875004	-2316.508712	1 (-268.1 cm ⁻¹)
B- ¹ PC1	-2317.458468	-2316.423504	-2316.062207	0
B- ¹ P1	-1181.847220	-1181.647059	-1181.453450	0
Rh ₂ (OAc) ₄	-1135.633535	-1135.331132	-1135.177759	0
B- ¹ PC3	-2317.443616	-2316.369383	-2316.010703	0
B- ¹ P3	-1181.820131	-1181.619528	-1181.428310	0

The total energies, enthalpies and free energies of the lowest conformers of all species shown in Scheme 8 and 9 and archive entries

Table S4

	$E_{\text{tot}} (E_h)_{\text{DCM}}$	$G_{298, \text{DCM}}$	$H_{298, \text{DCM}}$	# of imaginary frequencies
M- ¹ INT1	-2279.326949	-2278.769389	-2278.414024	0
M- ¹ TS1	-2279.319339	-2278.763927	-2278.407256	1 (-29.3 cm ⁻¹)
M- ¹ INT2	-2279.367803	-2278.817103	-2278.459172	0
M- ¹ INT3	-2279.358364	-2278.792346	-2278.438568	0
M- ¹ INT4	-2279.356106	-2278.807825	-2278.445041	0
M- ¹ TS2	-2279.349229	-2278.799589	-2278.437235	1 (-97.6 cm ⁻¹)
M- ¹ TS3	-2279.342981	-2278.791988	-2278.433384	1 (-237.6 cm ⁻¹)
M- ¹ INT5	-2279.371186	-2278.825836	-2279.371186	0
M- ¹ INT6	-2279.383976	-2278.835815	-2278.472546	0
M- ¹ TS4	-2279.349363	-2278.799277	-2278.440057	1 (-267.5 cm ⁻¹)
M- ¹ TS5	-2279.329842	-2278.774218	-2278.412747	1 (-417.6 cm ⁻¹)
M- ¹ INT5.H ₂ O	-2355.753300	-2354.662007	-2354.280030	0
M- ¹ INT6.H ₂ O	-2355.843270	-2355.249845	-2354.866238	0
M- ¹ TS7	-2355.828958	-2355.243552	-2354.854588	1 (-148.8 cm ⁻¹)
M- ¹ INT7	-2355.861750	-2355.281500	-2354.890872	0
M- ¹ INT8	-2355.800079	-2355.238433	-2354.837042	0

M- ¹ PC3	-2279.417396	-2279.060454	-2278.941454	0
M- ¹ PC4	-2279.425781	-2279.070980	-2278.949357	0
Mf- ¹ INT4	-3211.677907	-3210.079472	-3209.281588	0
Mf- ¹ TS2	-3210.874817	-3210.071335	-3209.273931	1 (-108.7 cm ⁻¹)
Mf- ¹ TS3	-3210.870379	-3210.066247	-3209.270533	1 (-240.3 cm ⁻¹)
Mf- ¹ INT5	-3210.895284	-3210.099144	-3209.298560	0
Mf- ¹ INT6	-3210.908308	-3210.104819	-3209.309000	0

The total energies, enthalpies and free energies of the lowest conformers of all species Shown in Scheme 11 and 12 and archive entries

Table S5

	E _{tot} (E _h) _{DCM}	G _{298,DCM}	H _{298,DCM}	# of imaginary frequencies
Bn- ¹ INT1	-2318.637295	-2318.066513	-2317.685883	0
Bn- ¹ TS1	-2318.629785	-2318.060257	-2317.677904	1 (-9.5 cm ⁻¹)
Bn- ¹ INT2	-2318.682847	-2318.118419	-2317.735541	0
Bn- ¹ TS2	-2318.666065	-2318.090923	-2317.710711	1 (-42.0 cm ⁻¹)
Bn- ¹ INT3	-2318.666829	-2318.106353	-2317.719429	0
Bn- ¹ TS4-1	-2318.672961	-2318.106071	-2317.722029	1 (-854.4 cm ⁻¹)
Bn- ¹ TS5-1	-2318.667385	-2318.102763	-2317.714955	1 (-188.1 cm ⁻¹)
Bn- ¹ PC1	-2318.741413	-2318.170791	-2317.664913	0
Bn- ¹ P1	-1183.105099	-1182.843083	-1182.631927	0
Rh ₂ (OAc) ₄	-1135.633535	-1135.331132	-1135.177759	0
Bn- ¹ PC2	-2318.724425	-2318.161979	-2317.772194	0
Bn- ¹ P2	-1183.097870	-1182.836973	-1182.625808	0
Bn- ¹ TS6	-2318.646272	-2318.070947	-2317.688918	1 (-766.3 cm ⁻¹)
Bn- ¹ TS7	-2318.653216	-2318.084344	-2317.697229	1 (-150.1 cm ⁻¹)

C-¹INT1

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C-¹TS1

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.277567\H,0,3.84993907,-4.78864597,-0.017515\H,0,2.52922907,-5.9862519
7,-0.268303\O,0,2.11037707,-4.22172397,0.787721\S,0,0.42005007,-4.1968

0297,0.718592\N,0,0.06976207,-2.67845097,0.024496\Rh,0,-1.73397493,-2.45030397,-0.735994\C,0,1.78081607,-1.84962297,-1.11846\C,0,2.18227007,-2.92891197,-1.607936\C,0,2.49862107,-4.31630397,-1.672482\C,0,3.27397907,-4.90256397,-2.869871\C,0,1.81208107,-5.18167597,-2.746664\H,0,3.98194707,-5.70059897,-2.625239\H,0,3.62386607,-4.19672297,-3.6261\H,0,1.11141207,-4.66476797,-3.403605\H,0,1.48416107,-6.16541097,-2.404307\O,0,0.02207707,-4.04319297,2.13304\O,0,0.01666707,-5.39980197,-0.046116\C,0,1.80233307,-0.43864097,-0.859736\C,0,1.41099307,0.08934503,0.392072\C,0,2.30090607,0.43615703,-1.857967\C,0,1.52107407,1.46374103,0.633555\H,0,1.01777007,-0.58965297,1.149258\C,0,2.40459807,1.80723403,-1.60318\H,0,2.60696907,0.02435803,-2.822855\C,0,2.01589507,2.32683603,-0.356791\H,0,1.22178007,1.86217103,1.607161\H,0,2.79481407,2.47258203,-2.378756\H,0,2.10211107,3.39905203,-0.159122\\Version=ES64L-G09RevD.01\State=1-A\HF=-2278.075558\RMSD=2.173e-09\Dipole=1.1926344,0.6318237,-2.7335101\Quadrupole=-3.8982963,10.5756664,-6.6773701,-0.4112141,-18.5236933,10.7679143\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-¹TS2

1\1\GINB-A754\SP\RBPW91\GenECP\C20H23N1O11Rh2S1\SI0C001\07-Mar-2018\0\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\\Title Card Required\\0,1\O,0,3.399785,0.447233,-1.450342\C,0,2.626584,-0.250914,-2.200736\O,0,1.448076,-0.66747,-1.898939\O,0,1.824596,2.630604,-0.429055\C,0,0.629012,2.525519,-0.881548\O,0,-0.105654,1.469611,-0.820093\O,0,1.948129,1.473838,2.237507\C,0,0.795265,1.023185,2.574109\O,0,0.027558,0.28009,1.857829\O,0,3.565386,-0.670445,1.204964\C,0,2.865674,-1.74748,1.233747\O,0,1.665382,-1.881769,0.798145\C,0,3.131398,-0.636673,-3.573954\C,0,3.49972,-2.97815,1.846662\C,0,0.023758,3.728634,-1.567607\C,0,0.272436,1.428564,3.937445\H,0,-1.027285,3.848385,-1.270069\H,0,0.600491,4.631925,-1.328766\H,0,0.045432,3.566738,-2.658034\H,0,1.104911,1.517505,4.649406\H,0,-0.213258,2.415395,3.858097\H,0,-0.467923,0.703018,4.299967\H,0,3.19089,-1.734022,-3.645583\H,0,2.415613,-0.299001,-4.339054\H,0,4.119196,-0.195176,-3.758504\H,0,3.3848,-3.834801,1.165735\H,0,4.562416,-2.797675,2.054411\H,0,2.980363,-3.229133,2.785572\Rh,0,2.698419,0.981323,0.396675\C,0,-2.771912,-3.47873,-0.087284\H,0,-3.490336,-4.307939,-0.190355\H,0,-1.773992,-3.898508,0.115866\O,0,-2.782241,-2.80619,-1.359562\S,0,-1.330879,-2.029216,-1.754142\N,0,-0.875207,-1.430977,-0.258433\Rh,0,0.66504,-0.256142,-0.041605\C,0,-3.210722,-2.517946,1.04221\C,0,-4.416225,-2.901518,1.916238\C,0,-3.024958,-2.984227,2.483369\H,0,-4.930527,-3.829824,1.649897\H,0,-5.072848,-2.097036,2.254827\H,0,-2.709177,-2.239013,3.216296\H,0,-2.574809,-3.972889,2.616256\O,0,-1.75236,-1.086806,-2.808003\O,0,-0.338743,-3.092792,-2.056286\C,0,-3.064514,-1.120008,0.716049\C,0,-3.274655,0.076676,0.473557\C,0,-3.551397,1.427605,0.155968\C,0,-3.572845,2.426285,1.166709\C,0,-3.863732,1.793179,-1.182252\C,0,-3.905297,3.745432,0.846591\H,0,-3.334953,2.145211,2.195219\C,0,-4.18765,3.117295,-1.488583\H,0,-3.827855,1.027433,

-1.959617\C,0,-4.214411,4.096584,-0.479242\H,0,-3.926198,4.505177,1.633068\H,0,-4.425249,3.388874,-2.520935\H,0,-4.477322,5.12944,-0.724542\
\Version=ES64L-G09RevD.01\State=1-A\HF=-2278.0845126\RMSD=5.144e-09\Dipole=-0.446475,1.6110174,2.6987027\Quadrupole=-4.9408456,8.3359521,-3.3951065,-11.5461368,-12.2088018,-15.2983771\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-¹INT2

1\1\GINB-A765\SP\RBPW91\GenECP\C20H23N1O11Rh2S1\SIOC001\07-Mar-2018\0\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\Title Card
Required\0,1\Rh,0,2.878984,0.64863,0.259682\Rh,0,0.588192,-0.069714,
-0.041354\O,0,2.183531,2.320282,1.227412\C,0,0.91836,2.447348,1.392287
\O,0,0.007047,1.637697,0.978142\O,0,2.922694,-0.356458,2.044183\C,0,1.
870767,-0.984636,2.417723\O,0,0.753253,-1.058386,1.78126\O,0,3.493344,
-1.044897,-0.715725\C,0,2.594807,-1.860928,-1.135937\O,0,1.32337,-1.73
7596,-0.993667\O,0,2.754676,1.621652,-1.540778\C,0,1.638068,1.604139,-
2.170508\O,0,0.561757,1.002925,-1.800186\N,0,-1.518836,-0.634664,-0.30
7221\C,0,0.443996,3.65486,2.178788\C,0,1.561422,2.387085,-3.466745\C,0
,1.943686,-1.719792,3.74404\C,0,3.071046,-3.07977,-1.900824\S,0,-2.114
127,-1.523455,-1.882421\O,0,-3.521123,-1.130549,-2.126478\O,0,-1.10242
5,-1.5481,-2.938523\C,0,-2.417888,-1.144825,0.765756\C,0,-2.658043,0.0
82178,0.358643\C,0,-3.283742,1.366835,0.273387\C,0,-2.823698,2.311119,
-0.674386\C,0,-4.380788,1.68312,1.111323\C,0,-3.461194,3.551153,-0.779
705\H,0,-1.969088,2.061078,-1.306449\C,0,-5.001222,2.929907,1.001694\H
,0,-4.736528,0.948483,1.838353\C,0,-4.546022,3.864862,0.05545\H,0,-3.1
08286,4.278744,-1.515427\H,0,-5.846868,3.173254,1.650515\H,0,-5.039094
,4.837038,-0.030647\C,0,-2.684022,-2.535327,1.119706\O,0,-2.088792,-3.
078208,-1.219844\C,0,-3.061862,-3.299031,-0.155003\H,0,-3.048508,-4.38
6777,0.013595\H,0,-4.06047,-2.997468,-0.51264\C,0,-3.319369,-2.915187,
2.446822\H,0,-4.032938,-3.744439,2.434185\H,0,-3.581808,-2.106436,3.13
3219\C,0,-1.860807,-3.215074,2.207612\H,0,-1.102569,-2.601183,2.694947
\H,0,-1.564913,-4.249973,2.015633\H,0,2.461875,-3.956488,-1.637832\H,0
,2.944896,-2.898613,-2.981122\H,0,4.132601,-3.272475,-1.695535\H,0,1.7
70588,-2.796099,3.584583\H,0,2.926503,-1.573514,4.210416\H,0,1.156143,
-1.352644,4.421326\H,0,0.939242,1.8521,-4.198374\H,0,1.093851,3.367511
, -3.274741\H,0,2.568807,2.555734,-3.870335\H,0,0.288009,3.36376,3.2312
93\H,0,1.199204,4.451878,2.148452\H,0,-0.515311,4.018119,1.783993\
\Version=ES64L-G09RevD.01\State=1-A\HF=-2278.1301712\RMSD=8.443e-10\Dipole
=-2.768247,-0.1695109,2.6621369\Quadrupole=-7.9879427,14.8728982,-6.88
49555,-5.2464558,-18.050852,-12.3629732\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-¹INT3

1\1\GINB-A764\SP\RBPW91\GenECP\C20H23N1O11Rh2S1\SIOC001\07-Mar-2018\0\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\Title Card
Required\0,1\C,0,-3.24498,-2.674951,1.047569\H,0,-3.763579,-3.131902

, 1.904315\H, 0, -3.065689, -3.453672, 0.287537\O, 0, -4.170469, -1.691641, 0.5
12658\S, 0, -3.766431, -1.293829, -1.080609\C, 0, -1.501754, -0.980304, 0.5301
82\Rh, 0, 0.508192, -0.101662, 0.048611\C, 0, -1.869291, 0.26753, 0.123674\N, 0
, -2.045267, -0.775088, -0.912114\C, 0, -2.374702, 1.597985, 0.328168\C, 0, -2.
413927, 2.167568, 1.624189\C, 0, -2.839214, 2.346809, -0.780211\C, 0, -2.92299
1, 3.456476, 1.803503\H, 0, -2.050712, 1.588781, 2.475561\C, 0, -3.346073, 3.63
4805, -0.588636\H, 0, -2.811681, 1.897038, -1.773282\C, 0, -3.389751, 4.192355
, 0.700215\H, 0, -2.96362, 3.889213, 2.806869\H, 0, -3.714525, 4.204663, -1.445
798\H, 0, -3.792665, 5.198548, 0.84657\C, 0, -1.926284, -2.032228, 1.491293\C,
0, -1.648657, -1.864178, 2.978356\C, 0, -0.983684, -2.982705, 2.212287\O, 0, -4
.649585, -0.170561, -1.424137\O, 0, -3.721914, -2.515459, -1.899682\O, 0, 2.77
4688, 2.077386, 0.475176\C, 0, 1.654194, 2.438323, 0.979423\O, 0, 0.55555, 1.76
7095, 0.951259\O, 0, 3.361909, -0.58625, 1.386994\C, 0, 2.404038, -0.922917, 2.
163051\O, 0, 1.145069, -0.84774, 1.896173\O, 0, 2.964177, -1.588152, -1.322521
\C, 0, 1.886984, -2.282513, -1.361419\O, 0, 0.74581, -1.949201, -0.870664\O, 0,
2.408551, 1.078854, -2.216639\C, 0, 1.168141, 1.154151, -2.530327\O, 0, 0.1778
51, 0.758138, -1.813029\C, 0, 1.613598, 3.768264, 1.703983\C, 0, 0.818533, 1.76
6841, -3.870717\C, 0, 2.77054, -1.461359, 3.532179\C, 0, 1.954078, -3.640571, -
2.029993\H, 0, 2.360638, -0.80173, 4.31404\H, 0, 2.326898, -2.459096, 3.678187
\H, 0, 3.861689, -1.521452, 3.637857\H, 0, 2.87024, -3.726432, -2.628982\H, 0, 1
.955932, -4.428856, -1.259156\H, 0, 1.066465, -3.793524, -2.660922\H, 0, 2.405
821, 4.429266, 1.327078\H, 0, 0.628201, 4.239569, 1.586877\H, 0, 1.786533, 3.59
9541, 2.780287\H, 0, 0.215565, 1.056354, -4.45699\H, 0, 0.207488, 2.67027, -3.7
1693\H, 0, 1.731187, 2.028163, -4.421748\Rh, 0, 2.880426, 0.241842, -0.418593\
H, 0, -1.014568, -1.026343, 3.274167\H, 0, -2.465213, -2.098976, 3.668257\H, 0,
0.079361, -2.891667, 1.997619\H, 0, -1.347665, -4.004999, 2.356975\\Version=
ES64L-G09RevD.01\State=1-A\HF=-2278.1201418\RMSD=5.880e-09\Dipole=1.43
12387, 0.5962732, 2.7524403\Quadrupole=-33.3137553, 20.7503728, 12.5633825
, -10.1265672, -9.4877165, -7.6261804\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-1TS3

1\1\GINB-A738\SP\RBPW91\GenECP\C20H23N1O11Rh2S1\SIOC001\08-Mar-2018\0\
\#p genecp scrf=(iefpcm, solvent=dichloromethane, smd) bpw91\\Title Card
Required\\0, 1\C, 0, -2.978638, -3.046942, 0.701979\H, 0, -3.386347, -3.88028
5, 1.294755\H, 0, -2.250889, -3.450279, -0.023043\O, 0, -4.110156, -2.461914, 0
.003421\S, 0, -3.657161, -1.566156, -1.383938\C, 0, -2.174436, -0.782741, 0.78
1442\Rh, 0, 0.704076, -0.015905, -0.03174\N, 0, -2.153092, -0.658964, -0.71494
5\C, 0, -2.507817, 0.40034, 0.306563\C, 0, -2.943473, 1.762174, 0.300923\C, 0, -
3.113828, 2.468653, 1.518232\C, 0, -3.225956, 2.406447, -0.927582\C, 0, -3.556
016, 3.793089, 1.498602\H, 0, -2.893176, 1.971324, 2.466049\C, 0, -3.68009, 3.7
28332, -0.931826\H, 0, -3.101788, 1.85288, -1.860084\C, 0, -3.844484, 4.425842
, 0.2762\H, 0, -3.68464, 4.334649, 2.439831\H, 0, -3.908267, 4.217329, -1.88265
7\H, 0, -4.199796, 5.459944, 0.267322\C, 0, -2.333523, -1.98513, 1.593936\C, 0,
-2.705321, -1.864629, 3.067286\C, 0, -1.351242, -2.400139, 2.686357\H, 0, -3.4
64604, -2.558644, 3.438573\H, 0, -2.763731, -0.859351, 3.491698\H, 0, -0.47585

3,-1.762373,2.814415\H,0,-1.165693,-3.473535,2.786617\O,0,-4.824819,-0.700961,-1.638963\O,0,-3.132747,-2.485721,-2.408855\O,0,2.882851,2.207006,-0.299501\C,0,1.694729,2.700119,-0.281741\O,0,0.60093,2.035875,-0.160122\O,0,3.131879,0.345208,1.905373\C,0,2.02035,0.307806,2.544318\O,0,0.85303,0.141923,2.026198\O,0,3.221454,-1.863944,-0.002323\C,0,2.130417,-2.540271,0.061332\O,0,0.939075,-2.056722,0.089506\O,0,2.981311,0.008327,-2.173909\C,0,1.815279,-0.100038,-2.709962\O,0,0.696314,-0.133651,-2.082648\C,0,1.56917,4.199794,-0.449033\C,0,1.754721,-0.167106,-4.220989\C,0,2.083902,0.509641,4.044801\C,0,2.260602,-4.049147,0.07018\H,0,3.088862,0.276311,4.421026\H,0,1.860464,1.564742,4.275788\H,0,1.331917,-0.11159,4.551979\H,0,2.181868,-4.421533,-0.964952\H,0,3.238489,-4.34743,0.471833\H,0,1.449203,-4.5035,0.655473\H,0,2.496786,4.700264,-0.140093\H,0,1.38675,4.429011,-1.51235\H,0,0.714226,4.578028,0.128573\H,0,2.691173,-0.57573,-4.624629\H,0,0.897164,-0.775838,-4.539422\H,0,1.619282,0.850981,-4.623091\Rh,0,3.085386,0.177591,-0.142427\Version=ES64L-G09RevD.01\State=1-A\HF=-2278.1130331\RMSD=9.719e-09\Dipole=1.2183422,0.8552436,2.9646756\Quadrupole=-33.1444289,22.5970119,10.547417,-12.0067261,-17.2575323,-11.0536465\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-INT4

1\1\GINB-A757\SP\RBPW91\GenECP\C20H23N1O11Rh2S1\SI0C001\07-Mar-2018\0\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\Title Card Required\0,1\C,0,-2.057826,-2.589225,1.589742\H,0,-2.291799,-3.172679,2.49404\H,0,-1.221274,-3.058096,1.05242\O,0,-3.260746,-2.659867,0.79461\O,0,-4.341445,-2.675676,-1.432071\S,0,-3.069793,-2.27209,-0.829804\O,0,-1.789757,-2.829631,-1.30803\N,0,-3.10833,-0.571748,-0.852478\C,0,-2.445869,0.198341,-0.011546\Rh,0,0.494316,0.034785,0.20904\Rh,0,2.783549,0.160054,-0.665105\O,0,0.955779,-1.932811,0.699622\O,0,3.084752,-1.791376,-0.138699\O,0,1.297826,0.651702,2.029043\C,0,2.564977,0.88044,2.123535\O,0,3.424381,0.772219,1.184743\O,0,0.304169,2.018779,-0.345905\O,0,2.433762,2.104474,-1.192674\O,0,-0.049921,-0.454783,-1.715423\C,0,0.842812,-0.617829,-2.628819\O,0,2.106676,-0.457792,-2.48794\C,0,0.322249,-1.031261,-3.987366\C,0,3.067889,1.30076,3.490165\C,0,-1.34389,-0.266867,0.857833\C,0,2.115924,-2.41719,0.413749\C,0,2.329891,-3.876364,0.760543\C,0,1.291251,2.613957,-0.926047\C,0,1.073383,4.068068,-1.291242\C,0,-2.833714,1.632809,0.000056\C,0,-2.292187,2.522287,0.953465\C,0,-3.827821,2.100967,-0.889653\C,0,-2.74104,3.847044,1.02312\H,0,-1.506924,2.176447,1.630228\C,0,-4.25848,3.428507,-0.829578\H,0,-4.255805,1.403899,-1.612977\C,0,-3.721221,4.305136,0.130101\H,0,-2.318529,4.523969,1.770873\H,0,-5.024539,3.781045,-1.525765\H,0,-4.069708,5.340653,0.182411\H,0,3.384536,-4.149333,0.625938\H,0,2.018309,-4.070869,1.79786\H,0,1.704839,-4.501207,0.10217\H,0,-0.346364,-1.897364,-3.873803\H,0,-0.270903,-0.209366,-4.41973\H,0,1.156882,-1.272115,-4.658464\H,0,1.415325,4.704357,-0.457716\H,0,1.665488,4.324795,-2.180524\H,0,0.007791,4.268393,-1.464248\H,0,3.087952,0.424329,4.158906\H,0,4.083605,1.7098

5,3.411331\H,0,2.391117,2.045131,3.935057\C,0,-1.691202,-1.156212,2.00
0534\C,0,-2.462389,-0.573369,3.189765\C,0,-1.023898,-1.016184,3.355243
\H,0,-3.268375,-1.186164,3.603627\H,0,-2.66927,0.499617,3.190877\H,0,-
0.256342,-0.247295,3.450304\H,0,-0.8218,-1.934886,3.91446\\Version=ES6
4L-G09RevD.01\State=1-A\HF=-2278.1404891\RMSD=6.237e-09\Dipole=1.28684
55,2.3689626,2.7556112\Quadrupole=-27.2215168,14.0134667,13.20805,-20.
7937425,-1.3237482,-8.9767385\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-¹Ts4

1\1\GINB-A755\SP\RBPW91\GenECP\C20H23N1O11Rh2S1\SIOC001\15-Mar-2018\0\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\\Title Card
Required\\0,1\C,0,-2.727878,-2.719722,1.242327\H,0,-3.071205,-3.33073
3,2.091314\H,0,-2.298574,-3.386472,0.476137\O,0,-3.924904,-2.08355,0.7
22461\S,0,-3.785827,-1.68092,-0.90376\C,0,-1.327263,-0.691652,0.665645
\Rh,0,0.582188,-0.080906,0.062781\C,0,-2.186121,0.204239,0.031066\N,0,
-2.313577,-0.800385,-0.920999\C,0,-2.718743,1.532462,0.131098\C,0,-2.4
27395,2.334132,1.264731\C,0,-3.564354,2.037163,-0.889149\C,0,-2.997151
,3.60206,1.385789\H,0,-1.751379,1.949876,2.031358\C,0,-4.127074,3.3084
09,-0.758075\H,0,-3.779919,1.414567,-1.758594\C,0,-3.849031,4.089558,0
.377572\H,0,-2.778685,4.217361,2.26268\H,0,-4.786738,3.693454,-1.53991
6\H,0,-4.294743,5.08346,0.476509\C,0,-1.691868,-1.700305,1.7068\C,0,-1
.768934,-1.236713,3.165332\C,0,-0.709611,-2.222681,2.736073\O,0,-4.952
161,-0.819298,-1.154799\O,0,-3.549337,-2.892871,-1.699087\O,0,2.538326
,2.271293,-0.704025\C,0,1.348151,2.687763,-0.484269\O,0,0.336287,1.962
478,-0.149863\O,0,3.320155,0.611978,1.523735\C,0,2.338255,0.562577,2.3
42073\O,0,1.110469,0.289171,2.054452\O,0,3.313551,-1.71534,-0.234628\C
,0,2.310838,-2.471755,0.018245\O,0,1.095585,-2.094588,0.209392\O,0,2.5
14112,-0.050748,-2.434834\C,0,1.294532,-0.28641,-2.754682\O,0,0.293883
, -0.355141,-1.94692\C,0,1.100065,4.1783,-0.597152\C,0,0.980142,-0.4777
61,-4.223412\C,0,2.629451,0.874491,3.797653\C,0,2.566837,-3.96463,0.07
9331\H,0,2.22148,1.867963,4.047244\H,0,2.136511,0.140219,4.452069\H,0,
3.71206,0.877776,3.979245\H,0,3.643178,-4.164345,0.163639\H,0,2.027308
, -4.412508,0.926492\H,0,2.186994,-4.434221,-0.843023\H,0,1.181177,4.63
6454,0.402888\H,0,1.852991,4.639301,-1.250547\H,0,0.087766,4.372277,-0
.977557\H,0,0.177776,-1.218293,-4.347512\H,0,0.626919,0.478215,-4.6449
06\H,0,1.88205,-0.787358,-4.768512\Rh,0,2.945637,0.280136,-0.463329\H,
0,-2.630468,-1.575405,3.748505\H,0,-1.434299,-0.221798,3.390126\H,0,-0
.813687,-3.271254,3.031771\H,0,0.314841,-1.860719,2.67339\\Version=ES6
4L-G09RevD.01\State=1-A\HF=-2278.1171841\RMSD=6.701e-09\Dipole=1.03918
8,1.8769213,2.5412546\Quadrupole=-32.8940003,20.7324112,12.1615891,-19
.8957146,-6.5336638,-6.8062579\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-¹PC1

1\1\GINB-A759\SP\RBPW91\GenECP\C20H23N1O11Rh2S1\SIOC001\20-Mar-2018\0\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\\Title Card
Required\\0,1\C,0,-1.063181,-2.874696,1.124576\H,0,-1.629634,-3.50453

8,1.840686\H,0,-0.032207,-3.256369,1.060772\O,0,-1.578367,-3.06477,-0.231975\S,0,-3.428223,-2.612292,-0.258457\N,0,-3.496587,-0.717259,-0.576735\C,0,-2.792066,0.072282,0.21824\Rh,0,0.655024,-0.149634,0.292601\Rh,0,2.713837,0.537838,-0.82396\O,0,1.872288,-0.855481,1.837854\O,0,3.811387,-0.292656,0.695339\O,0,0.672625,1.722651,1.211366\C,0,1.678119,2.547215,1.011614\O,0,2.673462,2.311774,0.203518\O,0,-0.352633,0.576498,-1.358021\O,0,1.598707,1.346841,-2.342853\O,0,0.914633,-1.961897,-0.668106\C,0,1.863646,-2.128477,-1.5566\O,0,2.766649,-1.227141,-1.849635\C,0,1.928843,-3.459275,-2.255364\C,0,1.659428,3.866657,1.738807\C,0,-1.786563,-0.283211,1.239118\C,0,3.179246,-0.806569,1.716448\C,0,4.001265,-1.407007,2.82735\C,0,0.302793,1.169788,-2.327927\C,0,-0.502078,1.674652,-3.493895\C,0,-3.218633,1.504984,0.082275\C,0,-2.337492,2.573926,0.369328\C,0,-4.540566,1.794872,-0.343919\C,0,-2.772981,3.902197,0.228083\H,0,-1.315929,2.364689,0.683534\C,0,-4.966051,3.12303,-0.484326\H,0,-5.219658,0.96774,-0.552208\C,0,-4.083737,4.182758,-0.198928\H,0,-2.085317,4.721225,0.451515\H,0,-5.988037,3.332059,-0.807394\H,0,-4.417478,5.217862,-0.302497\H,0,3.918432,-2.506242,2.798604\H,0,5.054958,-1.124735,2.712633\H,0,3.623121,-1.071551,3.804322\H,0,2.419369,-3.348273,-3.231289\H,0,2.520523,-4.168125,-1.651123\H,0,0.917279,-3.869856,-2.37358\H,0,0.152299,2.178991,-4.215156\H,0,-1.014017,0.830753,-3.982992\H,0,-1.280426,2.368076,-3.140269\H,0,2.686775,4.184559,1.962697\H,0,1.201429,4.637481,1.095942\H,0,1.073333,3.79049,2.663785\C,0,-1.628522,0.346912,2.642309\C,0,-1.105349,-1.465581,1.612197\C,0,-0.893357,-0.983409,3.053945\H,0,-1.025811,1.26045,2.706637\H,0,-2.594119,0.497333,3.15119\H,0,0.151496,-0.886158,3.376944\H,0,-1.455623,-1.588801,3.784869\O,0,-4.022334,-3.310965,-1.591723\O,0,-4.039971,-2.967984,1.222484\\Version=ES64L-G09RevD.01\State=1-A\HF=-2278.1210822\RMSD=3.979e-09\Dipole=2.419495,2.943369,2.1004318\Quadrupole=-19.7469429,10.3548286,9.3921143,-34.3827843,4.5817409,-4.3003945\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-1PC2

1\1\GINB-A754\SP\RBPW91\GenECP\C20H23N1O11Rh2S1\SIOC001\20-Mar-2018\0\ \#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\Title Card Required\0,1\C,0,3.122771,2.649753,-0.82566\H,0,3.528304,3.023899,0.127352\H,0,3.708864,3.062515,-1.65927\N,0,0.665817,1.142161,0.258131\S,0,0.753776,2.947191,0.242249\O,0,1.780276,3.182113,-1.031698\C,0,2.088167,0.481445,-1.831812\H,0,2.365571,-0.455337,-2.317495\H,0,1.502369,1.171301,-2.443388\O,0,1.406548,3.326422,1.508304\O,0,-0.516629,3.512888,-0.189197\C,0,3.093534,1.121614,-0.862338\C,0,4.361261,0.504904,-0.586416\C,0,5.460879,0.023126,-0.332294\C,0,6.73683,-0.540532,-0.032431\C,0,7.175068,-1.725027,-0.676115\C,0,7.589516,0.07778,0.916697\C,0,8.427413,-2.270687,-0.374879\H,0,6.52257,-2.204824,-1.409592\C,0,8.841396,-0.474495,1.207145\H,0,7.255636,0.989764,1.417441\C,0,9.265128,-1.649104,0.565042\H,0,8.752588,-3.185487,-0.878278\H,0,9.489205,0.013568,1.940754\H,0,10.243842,-2.078274,0.796418\Rh,0,-1.315699,0.03933,0.0066

51\rh,0,-3.361253,-1.225582,0.127951\o,0,-0.477563,-1.30727,1.340123\C
,0,-1.206929,-2.287455,1.755216\o,0,-2.424141,-2.512869,1.430349\o,0,-
0.753755,-1.16513,-1.581386\C,0,-1.572635,-2.077836,-1.973679\o,0,-2.7
16038,-2.350192,-1.459342\o,0,-2.257405,1.28462,-1.331646\C,0,-3.49101
,1.064799,-1.616003\o,0,-4.218356,0.105228,-1.167161\o,0,-1.975374,1.1
41172,1.614169\C,0,-3.133467,0.872078,2.110533\o,0,-3.933877,-0.044744
,1.707423\C,0,-0.544226,-3.267179,2.703468\C,0,-3.590716,1.741919,3.26
3351\C,0,-1.14768,-2.895264,-3.178609\C,0,-4.158552,2.055602,-2.548073
\C,0,1.801389,0.431015,-0.367444\H,0,1.930297,-0.531512,0.131209\H,0,0
.720656,0.960004,1.272762\H,0,-0.049116,-2.724742,3.523355\H,0,-1.2842
95,-3.968537,3.109924\H,0,0.233041,-3.833307,2.164338\H,0,-0.086976,-3
.174903,-3.095678\H,0,-1.770766,-3.794333,-3.272465\H,0,-1.26203,-2.28
5935,-4.090513\H,0,-2.77746,1.860853,3.994769\H,0,-3.842105,2.745671,2
.883196\H,0,-4.475888,1.307317,3.745829\H,0,-3.425234,2.473516,-3.2515
72\H,0,-4.985086,1.57566,-3.089908\H,0,-4.570589,2.887658,-1.952898\\V
ersion=ES64L-G09RevD.01\State=1-A\HF=-2278.159086\RMSD=7.381e-10\Dipol
e=2.6206067,-1.0188721,-0.3140008\Quadrupole=6.0013963,-9.9682355,3.96
68393,-11.1793337,0.7991918,0.4352464\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-1PC3

1\1\GINB-A733\SP\RBPW91\GenECP\C20H23N1O11Rh2S1\SIOC001\20-Mar-2018\0\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\Title Card
Required\0,1\rh,0,-2.609429,0.002817,-0.978376\o,0,-2.135625,-1.8312
39,-1.771922\C,0,-1.035771,-2.426234,-1.39014\o,0,-0.17313,-1.936244,-
0.528347\o,0,-3.697078,-0.917083,0.484856\C,0,-3.068104,-1.28996,1.563
865\o,0,-1.785612,-1.105582,1.775372\o,0,-3.023708,1.835036,-0.154665\
C,0,-2.232422,2.298789,0.776963\o,0,-1.175001,1.669568,1.235461\o,0,-1
.598246,0.928914,-2.483298\C,0,-0.32063,1.156037,-2.322795\o,0,0.34906
8,0.823811,-1.242314\N,0,3.371187,0.928237,-0.423959\C,0,-0.745616,-3.
792099,-1.956607\C,0,0.441626,1.819595,-3.431991\C,0,-3.864131,-1.9572
68,2.655309\C,0,-2.534113,3.652491,1.359111\S,0,3.01749,2.841905,-0.15
542\o,0,4.257476,3.440075,0.719637\o,0,2.592169,3.574002,-1.54335\C,0,
2.670983,0.076312,0.302966\o,0,1.45764,2.838905,0.912399\C,0,1.628916,
1.773922,1.922866\H,0,0.763741,1.900108,2.584459\H,0,2.557963,1.963092
,2.497416\C,0,1.659547,0.363323,1.34319\rh,0,-0.569099,-0.108238,0.373
776\H,0,1.104101,1.085723,-3.920922\H,0,-0.255849,2.224562,-4.175667\H
,0,1.082727,2.61259,-3.016772\H,0,0.318257,-4.033844,-1.842003\H,0,-1.
339643,-4.548771,-1.416608\H,0,-1.039176,-3.830181,-3.015049\H,0,-4.83
0927,-2.294505,2.261132\H,0,-3.305446,-2.808037,3.071193\H,0,-4.044968
, -1.241161,3.474382\H,0,-1.765023,4.368863,1.026979\H,0,-3.52157,3.996
197,1.0277\H,0,-2.495648,3.61182,2.457938\C,0,3.159475,-1.316547,-0.00
2885\C,0,3.014046,-1.853497,-1.2997\C,0,3.902564,-2.026345,0.967815\C,
0,3.568293,-3.107307,-1.607643\H,0,2.467897,-1.282572,-2.049684\C,0,4.
457777,-3.277132,0.654311\H,0,4.070805,-1.583827,1.952027\C,0,4.287057
, -3.822681,-0.632466\H,0,3.45434,-3.517121,-2.613658\H,0,5.037298,-3.8

16493,1.40676\H,0,4.726632,-4.792221,-0.877013\C,0,0.962646,-0.626422,
2.039373\C,0,0.510716,-0.845653,3.447081\C,0,1.006327,-2.017377,2.5635
5\H,0,1.155707,-0.473851,4.249519\H,0,-0.557594,-0.825947,3.663779\H,0
,1.973537,-2.482247,2.7613\H,0,0.23969,-2.709371,2.210579\\Version=ES6
4L-G09RevD.01\State=1-A\HF=-2278.1051945\RMSD=7.019e-09\Dipole=-1.7369
373,-4.2408795,2.1096916\Quadrupole=-17.1737014,-0.0302426,17.203944,-
27.450955,-4.5063879,4.7159154\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-1P1

1\1\GINB-A758\SP\RBPW91\6-311++G(d,p)\C12H11N1O3S1\SIOC001\27-Mar-2018
\0\#p 6-311++g(d,p) bpw91 scrf=(iefpcm,solvent=dichloromethane,smd)\
Title Card Required\\0,1\C,0,2.756998,1.287461,-0.610488\H,0,3.514409,
1.257202,0.199308\H,0,3.148041,1.949975,-1.404736\O,0,2.638944,-0.0128
67,-1.271483\S,0,2.155552,-1.327183,0.053542\N,0,0.219518,-1.308332,-0
.087918\C,0,-0.359369,-0.120351,-0.00558\C,0,0.221378,1.210826,0.13606
4\C,0,-1.855477,-0.239709,-0.033835\C,0,-2.631768,0.651907,-0.811651\C
,0,-2.49516,-1.280198,0.680492\C,0,-4.027482,0.509358,-0.861556\H,0,-2
.14037,1.430555,-1.397662\C,0,-3.891527,-1.410575,0.633937\H,0,-1.8880
1,-1.969688,1.268347\C,0,-4.660442,-0.517077,-0.135238\H,0,-4.619807,1
.194903,-1.471267\H,0,-4.379164,-2.209476,1.196144\H,0,-5.746981,-0.62
1517,-0.171609\C,0,-0.373172,2.502664,0.731078\C,0,1.462758,1.775523,-
0.071686\C,0,1.060452,3.130591,0.50582\H,0,-1.176573,2.98375,0.154573\
H,0,-0.684363,2.427012,1.784387\H,0,1.096157,3.978876,-0.197305\H,0,1.
589961,3.413058,1.430323\O,0,2.630274,-2.754586,-0.541466\O,0,2.733047
, -0.788036,1.490962\\Version=ES64L-G09RevD.01\State=1-A\HF=-1142.50288
98\RMSD=7.109e-09\Dipole=-2.5239536,3.7181018,0.0943291\Quadrupole=4.4
426944,0.5161346,-4.958829,15.1619277,-0.487941,-4.888707\PG=C01 [X(C1
2H11N1O3S1)]\@

C-1P2

1\1\GINB-OM103\SP\RBPW91\6-311++G(d,p)\C12H11N1O3S1\WEIY\19-May-2018\
\0\#p 6-311++g(d,p) bpw91 scrf=(iefpcm,solvent=dichloromethane,smd)\Ti
tle Card Required\\0,1\C,0,-1.479108,-0.01221,1.437979\H,0,-1.182897,-
1.066426,1.310208\H,0,-1.208069,0.31883,2.453074\N,0,-2.976682,0.83851
8,-1.185412\S,0,-3.553975,-0.684518,-0.199144\O,0,-2.947456,0.11231,1.
40455\C,0,-1.321333,2.276028,0.111405\H,0,-0.597565,3.062585,-0.106389
\H,0,-2.196772,2.574358,0.691158\O,0,-2.702942,-2.068991,-0.437996\O,0
, -5.174375,-0.694182,-0.170644\C,0,-0.802246,0.859545,0.367047\C,0,0.6
05369,0.588042,0.225843\C,0,1.805998,0.33531,0.130388\C,0,3.198382,0.0
28934,0.027041\C,0,4.167707,1.065713,-0.046221\C,0,3.636886,-1.322915,
-0.00152\C,0,5.531668,0.754861,-0.144705\H,0,3.837155,2.10593,-0.02268
2\C,0,5.003341,-1.622431,-0.09806\H,0,2.896382,-2.123097,0.052533\C,0,
5.954896,-0.587477,-0.170273\H,0,6.266699,1.561043,-0.199637\H,0,5.327
124,-2.66545,-0.118048\H,0,7.018227,-0.825209,-0.245812\C,0,-1.590473,
1.223677,-0.951507\H,0,-0.963088,1.211792,-1.845465\H,0,-3.165152,0.61
2767,-2.176542\\Version=ES64L-G16RevA.03\State=1-A\HF=-1142.4635765\RM

SD=4.454e-09\Dipole=2.6290722,1.5361388,-0.747147\Quadrupole=-10.08149
64,4.4609635,5.6205329,-8.1679823,4.3496403,-2.416663\PG=C01 [X(C12H11
N1O3S1)]\@

C-1P3

1\1\GINB-A758\SP\RBPW91\6-311++G(d,p)\C12H11N1O3S1\SIOC001\27-Mar-2018
\0\#p 6-311++g(d,p) bpw91 scrf=(iefpcm,solvent=dichloromethane,smd)\
Title Card Required\0,1\N,0,0.761,-1.281431,0.087633\S,0,2.681717,-0.
923286,-0.04792\O,0,3.382035,-1.413041,1.338418\O,0,3.216313,-1.448036
, -1.486817\C,0,-0.040764,-0.230838,0.138154\O,0,2.760641,0.97658,-0.14
5355\C,0,1.733666,1.485092,0.804319\H,0,1.92613,2.565032,0.866373\H,0,
1.893983,1.035305,1.800856\C,0,0.350087,1.192895,0.260729\C,0,-1.48306
2,-0.628958,0.108964\C,0,-1.907252,-1.66069,-0.76232\C,0,-2.41617,-0.0
36755,0.993331\C,0,-3.24852,-2.07318,-0.765162\H,0,-1.179219,-2.121098
, -1.431505\C,0,-3.753858,-0.461817,0.992835\H,0,-2.085012,0.735262,1.6
9016\C,0,-4.174106,-1.476269,0.111191\H,0,-3.570623,-2.860977,-1.44902
9\H,0,-4.466309,-0.008078,1.685158\H,0,-5.216616,-1.801868,0.110818\C,
0,-0.437732,2.192779,-0.183711\C,0,-0.538985,3.652533,-0.426944\C,0,-1
.649598,2.66582,-0.886048\H,0,-0.764637,4.317662,0.412299\H,0,0.106093
,4.10467,-1.186106\H,0,-2.604319,2.680122,-0.353908\H,0,-1.748088,2.44
886,-1.953829\Version=ES64L-G09RevD.01\State=1-A\HF=-1142.4873376\RMS
D=5.426e-09\Dipole=-4.4146832,2.8759889,0.4398554\Quadrupole=-7.524793
9,7.8159696,-0.2911757,9.5371014,1.6046004,4.1027658\PG=C01 [X(C12H11N
1O3S1)]\@

C-1TS5

1\1\GINB-A765\SP\RBPW91\GenECP\C20H23N1O11Rh2S1\SIOC001\07-Mar-2018\0\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\Title Card
Required\0,1\C,0,-2.972554,-2.311434,1.850038\H,0,-3.538256,-2.20335
6,2.791909\H,0,-2.561424,-3.340018,1.821558\O,0,-3.920029,-2.114232,0.
809216\O,0,-4.336281,-2.521419,-1.644603\S,0,-3.225174,-2.147928,-0.76
6976\O,0,-2.005882,-2.979525,-0.690669\N,0,-2.994678,-0.497407,-0.9848
65\C,0,-2.426568,0.202842,-0.009778\Rh,0,0.534465,0.004868,0.200577\Rh
,0,2.828925,0.113402,-0.638394\O,0,1.016934,-1.917972,0.843475\O,0,3.1
70336,-1.774571,0.070947\O,0,1.240105,0.809785,1.98017\C,0,2.496184,1.
111325,2.070981\O,0,3.380417,0.932308,1.168655\O,0,0.311936,1.924895,-
0.546104\O,0,2.451878,1.98368,-1.368226\O,0,0.024605,-0.73768,-1.64629
4\C,0,0.938066,-0.944348,-2.528564\O,0,2.191999,-0.700724,-2.39932\C,0
,0.46924,-1.534967,-3.841675\C,0,2.939623,1.747481,3.374354\C,0,-1.447
372,-0.336428,0.958767\C,0,2.195159,-2.390614,0.62518\C,0,2.432518,-3.
826487,1.050875\C,0,1.285907,2.479754,-1.180531\C,0,1.004876,3.840119,
-1.786627\C,0,-2.779654,1.647203,0.011818\C,0,-2.124177,2.5949,0.83049
6\C,0,-3.88586,2.076406,-0.762502\C,0,-2.568281,3.921574,0.882765\H,0,
-1.242393,2.304869,1.399584\C,0,-4.315407,3.405185,-0.72029\H,0,-4.403
792,1.341443,-1.381153\C,0,-3.663147,4.333644,0.108032\H,0,-2.048142,4
.639113,1.523892\H,0,-5.172511,3.714993,-1.324671\H,0,-4.008577,5.3705

99,0.15164\H,0,1.9074,-4.499909,0.353755\H,0,3.505452,-4.058632,1.0345
71\H,0,2.02074,-4.004658,2.055524\H,0,1.317156,-1.674144,-4.524717\H,0
, -0.026891,-2.499657,-3.653461\H,0,-0.276945,-0.86855,-4.301948\H,0,1.
93829,4.408013,-1.900989\H,0,0.558348,3.701144,-2.785511\H,0,0.284395,
4.395919,-1.171036\H,0,4.030513,1.866876,3.389359\H,0,2.464358,2.73588
2,3.484799\H,0,2.620036,1.129998,4.228252\C,0,-1.545217,-0.012116,2.84
2573\C,0,-1.747957,-1.413345,1.835877\C,0,-0.931442,-1.391329,3.073219
\H,0,-2.518158,0.239023,3.274393\H,0,-0.802593,0.790188,2.80566\H,0,0.
154283,-1.402579,2.965609\H,0,-1.320105,-1.992523,3.902395\\Version=ES
64L-G09RevD.01\State=1-A\HF=-2278.1238329\RMSD=4.998e-09\Dipole=0.1889
882,1.7462009,4.3304889\Quadrupole=-28.7354769,10.3936893,18.3417876,-
15.5898088,-9.7065269,-10.3278015\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-¹TS6

1\1\GINB-A757\SP\RBPW91\GenECP\C20H23N1O11Rh2S1\SIOC001\07-Mar-2018\0\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\\Title Card
Required\\0,1\C,0,3.225594,2.639686,0.167409\O,0,2.175366,2.784837,-0
.809085\S,0,0.584904,2.706936,-0.235559\O,0,-0.20709,3.495864,-1.18683
7\O,0,0.600115,3.076606,1.199557\N,0,0.257058,1.086067,-0.542471\Rh,0,
-1.45129,0.079828,-0.133385\O,0,-1.895608,0.168648,-2.154891\C,0,-2.95
714,-0.4018,-2.597812\C,0,-3.198249,-0.314773,-4.089877\O,0,-2.585094,
1.759539,0.221583\C,0,-3.850656,1.62778,0.407162\C,0,-4.632874,2.90794
3,0.607483\Rh,0,-3.47109,-1.211434,0.10491\O,0,-3.816841,-1.050176,-1.
896464\O,0,-1.173801,-0.132519,1.8922\C,0,-2.055014,-0.770749,2.579605
\C,0,-1.83284,-0.826066,4.075935\O,0,-0.42891,-1.685607,-0.450281\C,0,
-1.095488,-2.788616,-0.424157\C,0,-0.299372,-4.061131,-0.63053\O,0,-4.
506681,0.522959,0.41814\O,0,-3.104083,-1.342234,2.111944\O,0,-2.355878
, -2.906761,-0.225653\H,0,3.019612,3.283341,1.03603\H,0,1.205084,0.5640
6,-0.570022\H,0,4.122466,3.009426,-0.349481\C,0,2.348446,0.164536,0.53
2676\H,0,-4.073137,3.593509,1.259844\H,0,-4.760544,3.407698,-0.366868\
H,0,-5.622209,2.691599,1.031599\H,0,-4.234573,-0.589939,-4.326222\H,0,
-2.978085,0.701273,-4.448049\H,0,-2.515858,-1.007437,-4.609497\H,0,-2.
057634,0.161594,4.511053\H,0,-2.489179,-1.577678,4.533663\H,0,-0.77935
, -1.053115,4.295765\H,0,-0.973551,-4.912066,-0.792707\H,0,0.381761,-3.
947282,-1.487025\H,0,0.316895,-4.256187,0.26258\C,0,3.467322,1.171682,
0.608806\C,0,2.63827,0.677284,1.8614\C,0,4.778959,0.639008,0.399961\C,
0,5.886422,0.142419,0.195076\C,0,7.16493,-0.437358,-0.033511\C,0,7.577
155,-1.581379,0.698837\C,0,8.046385,0.109065,-1.002491\C,0,8.829199,-2
.156923,0.463823\H,0,6.902501,-2.005222,1.44655\C,0,9.296545,-0.474982
, -1.227694\H,0,7.733089,0.988202,-1.570431\C,0,9.693007,-1.608106,-0.4
98304\H,0,9.133946,-3.038835,1.03418\H,0,9.965609,-0.045048,-1.978242\
H,0,10.671191,-2.061921,-0.679291\H,0,2.476408,-0.875248,0.21836\H,0,2
.011312,1.483402,2.261811\H,0,3.097904,0.020335,2.609524\\Version=ES64
L-G09RevD.01\State=1-A\HF=-2278.067373\RMSD=4.421e-09\Dipole=2.5507518
, -2.4496459,1.0292491\Quadrupole=20.5608194,-18.3608312,-2.1999882,-12

.9987866,1.3639746,2.185406\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-¹Ts7

1\1\GINB-A752\SP\RBPW91\GenECP\C20H23N1O11Rh2S1\SIOC001\07-Mar-2018\0\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\Title Card
Required\0,1\O,0,-2.939985,-2.57459,0.976281\O,0,-4.892021,-2.598115
, -0.619512\S,0,-3.466276,-2.276654,-0.689474\O,0,-2.553717,-3.019161,-
1.571511\N,0,-3.303545,-0.639999,-0.843898\C,0,-2.557296,0.117659,-0.0
57777\Rh,0,0.5494,-0.057137,0.14207\Rh,0,2.871653,0.167267,-0.588064\O
,0,0.40826,-1.670211,-1.120501\O,0,2.56116,-1.416332,-1.862509\O,0,1.2
49822,-1.347189,1.622267\C,0,2.514031,-1.603724,1.673604\O,0,3.419647,
-1.131268,0.905145\O,0,0.899262,1.557083,1.410019\O,0,3.078228,1.74108
2,0.713023\O,0,0.055342,1.209334,-1.414404\C,0,0.989828,1.675666,-2.16
7952\O,0,2.246612,1.452872,-2.051944\C,0,0.54186,2.559827,-3.314828\C,
0,2.957451,-2.57404,2.753524\C,0,-1.460464,-0.300931,0.856596\C,0,-1.6
4791,-2.175631,1.156547\C,0,1.424229,-2.002804,-1.846282\C,0,1.242761,
-3.210664,-2.741783\C,0,2.069439,2.101747,1.41069\C,0,2.258386,3.30980
5,2.309558\C,0,-2.839301,1.57656,-0.145714\C,0,-2.072321,2.529754,0.56
1519\C,0,-3.951386,2.018976,-0.90161\C,0,-2.419002,3.886322,0.520385\H
,0,-1.182843,2.222528,1.114515\C,0,-4.283592,3.375056,-0.947623\H,0,-4
.55044,1.280271,-1.436913\C,0,-3.521208,4.315352,-0.233599\H,0,-1.8144
3,4.612814,1.070745\H,0,-5.146704,3.700209,-1.535101\H,0,-3.786329,5.3
76126,-0.26592\H,0,1.697426,-3.018471,-3.724631\H,0,1.764958,-4.074898
, -2.298238\H,0,0.177854,-3.452735,-2.850724\H,0,0.053114,1.937582,-4.0
82534\H,0,-0.199283,3.292335,-2.962728\H,0,1.403195,3.072016,-3.763287
\H,0,2.058704,4.226541,1.72949\H,0,1.562931,3.280477,3.159726\H,0,3.29
6558,3.356868,2.666707\H,0,2.589916,-2.241641,3.736842\H,0,2.52765,-3.
570013,2.557944\H,0,4.052223,-2.650432,2.77304\C,0,-1.714715,-0.412466
,2.214319\C,0,-2.689941,-0.256223,3.310107\C,0,-1.17559,-0.402161,3.58
1467\H,0,-3.325519,-1.11176,3.564737\H,0,-3.185045,0.715468,3.415846\H
,0,-0.577476,0.472049,3.857904\H,0,-0.840279,-1.333501,4.048861\H,0,-1
.225455,-2.573423,2.085394\H,0,-0.965286,-2.364325,0.309185\Version=ES
S64L-G09RevD.01\State=1-A\HF=-2278.0982163\RMSD=1.820e-09\Dipole=0.182
9828,1.7254884,3.2180456\Quadrupole=-29.5417167,12.5488867,16.9928299,
-21.8476209,-2.7547626,-7.1761433\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-³INT1

1\1\GINB-A753\SP\UBPW91\GenECP\C20H23N1O11Rh2S1(3)\SIOC001\01-Mar-2018
\0\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\Title C
ard Required\0,3\Rh,0,-2.754861,-1.66809,0.092991\Rh,0,-1.668241,0.48
0132,0.055645\O,0,-4.326407,-0.803724,1.069281\C,0,-4.279849,0.450742,
1.337031\O,0,-3.305156,1.240483,1.051981\O,0,-3.637668,-1.251539,-1.69
9157\C,0,-3.386506,-0.110861,-2.234356\O,0,-2.631055,0.805256,-1.74040
4\O,0,-1.17112,-2.503372,-0.88459\C,0,-0.20303,-1.721379,-1.204597\O,0
, -0.130397,-0.467078,-0.935746\O,0,-1.85972,-2.063034,1.888198\C,0,-1.

078712,-1.176259,2.38714\O,0,-0.806091,-0.031342,1.865563\N,0,-0.72735
2,2.15873,-0.0399\C,0,-5.475552,1.069851,2.023886\C,0,-0.39815,-1.4979
85,3.699332\C,0,-4.019238,0.19765,-3.572522\C,0,0.952922,-2.304344,-1.
983897\S,0,0.536154,2.779679,-0.890067\O,0,0.470592,2.441542,-2.322828
\O,0,0.692267,4.188741,-0.457579\O,0,1.849147,1.90871,-0.33803\C,0,2.4
18541,2.284552,0.951919\H,0,1.991738,3.245065,1.277916\H,0,2.148162,1.
493844,1.668282\C,0,3.927954,2.411565,0.809352\C,0,4.454587,3.720939,0
.211853\C,0,4.602153,3.485008,1.687023\H,0,3.695743,4.427673,-0.134165
\H,0,5.343871,3.651672,-0.41755\H,0,5.58939,3.237884,2.082934\H,0,3.95
7761,4.037848,2.376456\C,0,4.649574,1.191445,0.549705\C,0,5.250462,0.1
44575,0.330609\C,0,5.953245,-1.066956,0.060151\C,0,7.216459,-1.042834,
-0.584012\C,0,5.402649,-2.321696,0.425825\C,0,7.899834,-2.233999,-0.85
0673\H,0,7.647094,-0.080493,-0.871146\C,0,6.092335,-3.507516,0.151002\
H,0,4.431773,-2.348428,0.927137\C,0,7.342631,-3.470534,-0.487051\H,0,8
.873182,-2.197025,-1.348435\H,0,5.652405,-4.46695,0.438575\H,0,7.87931
8,-4.399289,-0.699642\H,0,0.910939,-3.401188,-1.967962\H,0,0.894395,-1
.95281,-3.026958\H,0,1.906521,-1.945283,-1.571048\H,0,-0.8301,-2.40533
7,4.14092\H,0,0.677932,-1.657159,3.522309\H,0,-0.498456,-0.650513,4.39
3572\H,0,-6.089779,0.291778,2.495924\H,0,-5.145325,1.807346,2.769217\H
,0,-6.086079,1.600686,1.274814\H,0,-4.510748,1.181386,-3.534996\H,0,-3
.231996,0.253371,-4.341333\H,0,-4.744161,-0.580835,-3.842916\Version=
ES64L-G09RevD.01\State=3-A\HF=-2278.0983838\S2=2.011206\S2-1=0.\S2A=2.
000057\RMSD=5.494e-09\Dipole=-1.1667193,-2.6795722,1.684936\Quadrupole
=18.6180653,-20.2410054,1.62294,-6.3553635,1.2806639,9.6097373\PG=C01
[X(C20H23N1O11Rh2S1)]\@

C-³TS1

1\1\GINB-A751\SP\UBPW91\GenECP\C20H23N1O11Rh2S1(3)\SIOC001\28-Feb-2018
\0\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\Title C
ard Required\0,3\O,0,2.958559,1.659806,-0.918364\C,0,1.896363,1.94562
8,-1.578726\O,0,0.751015,1.377346,-1.444711\O,0,2.300807,1.527934,1.88
8847\C,0,1.049724,1.749703,2.068641\O,0,0.082651,1.210101,1.414404\O,0
,2.745502,-1.340717,1.836592\C,0,1.613369,-1.928082,1.979597\O,0,0.529
947,-1.647913,1.347956\O,0,3.376493,-1.190759,-0.972808\C,0,2.422363,-
1.728281,-1.643846\O,0,1.167563,-1.493056,-1.499495\C,0,1.986182,3.049
32,-2.609647\C,0,2.790241,-2.741011,-2.706012\C,0,0.66182,2.719118,3.1
65073\C,0,1.530799,-3.056579,2.986066\H,0,0.271823,2.15391,4.027722\H,
0,1.534418,3.302773,3.486381\H,0,-0.138972,3.384843,2.812459\H,0,2.513
193,-3.237035,3.441039\H,0,0.800744,-2.80192,3.770552\H,0,1.174043,-3.
97069,2.486801\H,0,1.286228,3.857381,-2.346089\H,0,3.009009,3.444567,-
2.657863\H,0,1.687381,2.659927,-3.595247\H,0,2.369863,-2.429254,-3.674
382\H,0,3.880795,-2.840529,-2.780754\H,0,2.340934,-3.714278,-2.45359\Rh
h,0,2.862521,0.167902,0.466037\C,0,-4.263792,-2.259997,-0.529819\H,0,-
5.322378,-2.117329,-0.797679\H,0,-4.017251,-3.334474,-0.573781\O,0,-3.
572511,-1.545009,-1.570389\S,0,-1.888403,-1.636711,-1.608634\N,0,-1.39

088,-0.448612,-0.532804\rh,0,0.52737,-0.148393,-0.076816\c,0,-2.974451
,0.60732,0.339513\c,0,-3.64855,-0.32,0.876045\c,0,-2.81057,2.012509,0.
065275\c,0,-3.2076,2.957597,1.044133\c,0,-2.337321,2.471617,-1.184596\
c,0,-3.132705,4.327522,0.772463\h,0,-3.576759,2.600161,2.008458\c,0,-2
.270775,3.845387,-1.445778\h,0,-2.024264,1.744379,-1.93491\c,0,-2.6646
46,4.77789,-0.473441\h,0,-3.445138,5.046905,1.535049\h,0,-1.912759,4.1
88364,-2.420687\h,0,-2.61062,5.849687,-0.684557\c,0,-3.984621,-1.71233
1,0.885439\c,0,-4.749896,-2.363143,2.047595\c,0,-3.282001,-2.620574,1.
9167\h,0,-5.447405,-3.160811,1.773234\h,0,-5.104952,-1.699251,2.838902
\h,0,-2.591847,-2.127595,2.602833\h,0,-2.939826,-3.583452,1.53012\o,0,
-1.585329,-1.216497,-2.989946\o,0,-1.513991,-2.987263,-1.128244\\Versi
on=ES64L-G09RevD.01\State=3-A\HF=-2278.0701403\S2=2.012295\S2-1=0.\S2A
=2.000087\RMSD=3.072e-09\Dipole=-0.2331348,0.7461136,2.4513574\Quadrup
ole=-6.2209124,10.4818997,-4.2609873,2.4756435,-17.7516732,-9.1838768\
PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-³TS2

1\1\GINB-A738\SP\UBPW91\GenECP\C20H23N1O11Rh2S1(3)\SIOC001\28-Feb-2018
\0\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\\Title C
ard Required\\0,3\o,0,-3.330689,-0.786468,-1.483766\c,0,-2.677817,0.06
4679,-2.190137\o,0,-1.550698,0.599436,-1.881564\o,0,-1.528894,-2.85118
4,-0.570872\c,0,-0.362606,-2.613978,-1.052687\o,0,0.265781,-1.493284,-
0.998855\o,0,-1.7022,-1.803078,2.125696\c,0,-0.582927,-1.274167,2.4560
91\o,0,0.110974,-0.456802,1.743053\o,0,-3.519887,0.250546,1.194454\c,0
, -2.903548,1.374456,1.268192\o,0,-1.713079,1.615689,0.847635\c,0,-3.28
6445,0.507542,-3.502381\c,0,-3.627843,2.53189,1.92245\c,0,0.342608,-3.
744123,-1.771018\c,0,-0.039706,-1.627115,3.826039\h,0,1.39087,-3.80267
8,-1.444466\h,0,-0.172408,-4.695849,-1.585691\h,0,0.343227,-3.537678,-
2.853821\h,0,-0.629872,-1.101117,4.594547\h,0,-0.150606,-2.70658,4.005
479\h,0,1.01262,-1.329944,3.921541\h,0,-3.717731,1.514296,-3.376611\h,
0,-2.506918,0.576118,-4.274522\h,0,-4.079335,-0.186526,-3.810828\h,0,-
3.55736,3.423669,1.282005\h,0,-4.679211,2.273016,2.103061\h,0,-3.14211
8,2.774482,2.881486\rh,0,-2.535458,-1.312366,0.320963\c,0,2.835255,3.6
84517,0.049431\h,0,3.901547,3.938933,-0.05617\h,0,2.263463,4.597784,0.
288311\o,0,2.48674,3.203011,-1.265692\s,0,0.912325,2.646193,-1.467559\
n,0,0.910263,1.298415,-0.479162\rh,0,-0.638269,0.12856,-0.098624\c,0,2
.741939,1.260478,0.610294\c,0,2.638998,2.614093,1.135125\c,0,3.158462,
2.920137,2.540603\c,0,1.674693,2.876323,2.288072\h,0,3.63756,3.894252,
2.683061\h,0,3.625091,2.100604,3.091765\h,0,1.104739,2.0192,2.650142\h
,0,1.118726,3.816844,2.250088\o,0,0.88508,2.281119,-2.894135\o,0,-0.00
6827,3.68205,-0.940751\c,0,3.324641,0.169444,0.417679\c,0,3.871383,-1.
084277,0.087997\c,0,4.636582,-1.240782,-1.104752\c,0,3.700156,-2.21112
4,0.943084\c,0,5.199565,-2.477669,-1.42297\h,0,4.765175,-0.380526,-1.7
65274\c,0,4.273713,-3.440461,0.613089\h,0,3.111103,-2.09574,1.855056\c
,0,5.024671,-3.581221,-0.568423\h,0,5.780152,-2.585531,-2.343327\h,0,4

.136907,-4.297439,1.27883\H,0,5.472005,-4.546442,-0.821154\\Version=ES64L-G09RevD.01\State=3-A\HF=-2278.0815667\S2=2.011403\S2-1=0.\S2A=2.000081\RMSD=2.604e-09\Dipole=0.9486438,-1.9409259,2.633374\Quadrupole=3.1180998,-0.8590685,-2.2590313,-12.5400459,6.6018356,16.2710886\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-³INT2

1\1\GINB-A750\SP\UBPW91\GenECP\C20H23N1O11Rh2S1(3)\SIOC001\01-Mar-2018\0\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\\Title Card Required\\0,3\O,0,3.348839,0.813518,-1.159269\C,0,2.419085,1.140878,-1.982243\O,0,1.163656,0.911656,-1.822365\O,0,2.567542,1.682889,1.47964\C,0,1.389076,2.194564,1.462462\O,0,0.353765,1.695687,0.888245\O,0,2.283985,-1.084186,2.286504\C,0,1.037129,-1.353571,2.442854\O,0,0.094381,-1.071037,1.618074\O,0,3.085411,-1.941648,-0.338831\C,0,2.082778,-2.41633,-0.988358\O,0,0.928737,-1.867327,-1.103498\C,0,2.820865,1.880026,-3.239257\C,0,2.262182,-3.749836,-1.680294\C,0,1.189814,3.49483,2.212871\C,0,0.635578,-2.067001,3.716707\H,0,0.348452,4.056982,1.786899\H,0,0.96029,3.27012,3.268084\H,0,2.111468,4.092829,2.186121\H,0,1.522203,-2.301958,4.319548\H,0,-0.047713,-1.429083,4.29962\H,0,0.094889,-2.993093,3.467851\H,0,2.575966,2.949134,-3.126499\H,0,3.900245,1.779626,-3.41319\H,0,2.255438,1.49515,-4.10027\H,0,3.30776,-4.078406,-1.618572\H,0,1.608538,-4.497228,-1.203179\H,0,1.949296,-3.666225,-2.731933\Rh,0,2.837838,-0.131061,0.574362\C,0,-4.558951,-1.887826,-0.594158\H,0,-5.553012,-1.602428,-0.971623\H,0,-4.510829,-2.983384,-0.474216\O,0,-3.680203,-1.462746,-1.662731\S,0,-2.032611,-1.66765,-1.420013\N,0,-1.540478,-0.19842,-0.645408\Rh,0,0.537882,-0.085876,-0.146992\C,0,-2.532484,0.61305,-0.070646\C,0,-3.650639,0.123442,0.540397\C,0,-2.370181,2.087534,-0.199836\C,0,-2.931855,2.953445,0.763167\C,0,-1.75071,2.640352,-1.340281\C,0,-2.877851,4.340835,0.589705\H,0,-3.408197,2.523748,1.648986\C,0,-1.697867,4.029883,-1.509744\H,0,-1.322828,1.972878,-2.090879\C,0,-2.25921,4.885443,-0.548574\H,0,-3.318556,4.999929,1.343594\H,0,-1.225375,4.446512,-2.404176\H,0,-2.221214,5.969848,-0.687396\C,0,-4.24358,-1.179353,0.731713\C,0,-5.182248,-1.456709,1.914\C,0,-3.79518,-2.021964,1.946518\H,0,-6.018265,-2.136789,1.722136\H,0,-5.424015,-0.609396,2.560253\H,0,-3.051658,-1.564767,2.601391\H,0,-3.6471,-3.087332,1.753928\O,0,-1.485763,-1.621549,-2.77976\O,0,-1.835674,-2.840668,-0.547524\\Version=ES64L-G09RevD.01\State=3-A\HF=-2278.1018661\S2=2.021403\S2-1=0.\S2A=2.000157\RMSD=2.416e-09\Dipole=-0.4894333,0.746313,2.0488073\Quadrupole=-1.481426,5.874901,-4.393475,5.8637479,-18.1825471,-6.4265151\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-³INT3

1\1\GINB-A753\SP\UBPW91\GenECP\C20H23N1O11Rh2S1(3)\SIOC001\01-Mar-2018\0\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\\Title Card Required\\0,3\O,0,-3.390634,-0.724264,-1.455208\C,0,-2.776468,0.177252,-2.135643\O,0,-1.656162,0.722092,-1.827441\O,0,-1.490921,-2.79449

5,-0.775126\C,0,-0.368578,-2.472219,-1.30743\O,0,0.215661,-1.330497,-1.20715\O,0,-1.623532,-1.97655,2.006534\C,0,-0.505334,-1.4396,2.333008\O,0,0.138988,-0.558545,1.652773\O,0,-3.520845,0.084548,1.299924\C,0,-2.936028,1.21962,1.441231\O,0,-1.767602,1.525463,1.004921\C,0,-3.411603,0.630414,-3.432503\C,0,-3.688085,2.312579,2.16862\C,0,0.322723,-3.51681,-2.157533\C,0,0.091573,-1.86141,3.659698\H,0,1.411331,-3.462981,-2.017914\H,0,-0.049758,-4.519146,-1.907482\H,0,0.106383,-3.31637,-3.220319\H,0,-0.06175,-2.938652,3.816845\H,0,1.16026,-1.615224,3.705016\H,0,-0.426578,-1.325202,4.472089\H,0,-2.890813,0.152687,-4.278824\H,0,-4.471494,0.344842,-3.460268\H,0,-3.300945,1.718581,-3.543355\H,0,-4.549926,1.895127,2.705622\H,0,-3.01481,2.834284,2.864219\H,0,-4.042665,3.054101,1.434132\Rh,0,-2.522116,-1.373454,0.272514\C,0,3.170757,3.415098,-0.87382\H,0,3.747395,3.163254,-1.778709\H,0,3.566486,4.350621,-0.442084\O,0,1.828511,3.654667,-1.381455\S,0,0.579391,3.189013,-0.374783\N,0,0.905696,1.493905,-0.283799\Rh,0,-0.696881,0.156667,-0.100701\C,0,2.251374,1.159926,-0.111662\C,0,3.235796,2.287245,0.149292\C,0,4.596203,2.004571,0.758562\C,0,3.522534,2.633512,1.608199\H,0,5.427338,2.632095,0.421751\H,0,4.869754,0.962822,0.940181\H,0,3.033077,2.017375,2.365563\H,0,3.591541,3.694357,1.862636\O,0,-0.619893,3.398721,-1.18262\O,0,0.73399,3.826814,0.945867\C,0,2.664569,-0.119828,-0.153585\C,0,3.475612,-1.24459,-0.167652\C,0,4.043335,-1.731339,-1.397114\C,0,3.7491,-1.989081,1.032117\C,0,4.836333,-2.876643,-1.408651\H,0,3.841045,-1.182103,-2.319474\C,0,4.544479,-3.131997,0.994874\H,0,3.319332,-1.638493,1.972705\C,0,5.094647,-3.587072,-0.219438\H,0,5.263357,-3.224105,-2.354124\H,0,4.741256,-3.679926,1.921109\H,0,5.716812,-4.485505,-0.239364\Version=ES64L-G09RevD.01\State=3-A\HF=-2278.1186202\S2=2.025447\S2-1=0.\S2A=2.00037\RMSD=2.376e-09\Dipole=2.200635,-1.9377418,0.3362695\Quadrupole=9.947057,-14.3421486,4.3950916,-5.8846883,0.5319491,3.8705098\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C⁻³TS3

1\1\GINB-A751\SP\UBPW91\GenECP\C20H23N1O11Rh2S1(3)\SIOC001\28-Feb-2018\O\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\Title Card Required\O,3\O,0,2.21047,2.589339,0.610452\C,0,0.950229,2.802259,0.465408\O,0,0.075974,1.91449,0.169825\O,0,2.542448,0.325758,2.378057\C,0,1.397306,-0.145863,2.714246\O,0,0.41704,-0.425131,1.928686\O,0,3.558346,-1.24347,0.143197\C,0,2.712555,-2.163624,-0.154744\O,0,1.447833,-1.994159,-0.290173\O,0,3.194433,1.013166,-1.621312\C,0,2.210602,0.77302,-2.415076\O,0,1.055108,0.318081,-2.08892\C,0,0.467411,4.219951,0.692567\C,0,2.423563,1.080915,-3.883696\C,0,1.185195,-0.429384,4.190087\C,0,3.255082,-3.556863,-0.392125\H,0,1.911747,0.12827,4.795762\H,0,0.159827,-0.164884,4.486764\H,0,1.326976,-1.506808,4.378415\H,0,2.552917,-4.311259,-0.009404\H,0,3.361319,-3.718437,-1.477748\H,0,4.239977,-3.674107,0.079283\H,0,0.436223,4.420891,1.776309\H,0,1.170481,4.935353,0.24153\H,0,-0.539843,4.356498,0.278368\H,0,2.012653,2.079895,-4.106209\H

,0,3.495342,1.083376,-4.123806\H,0,1.888444,0.34954,-4.505376\Rh,0,2.91644,0.684982,0.384994\C,0,-2.458914,-3.308477,-0.224482\H,0,-2.927285,-4.30463,-0.172678\H,0,-1.388089,-3.425463,-0.463939\O,0,-3.130876,-2.600863,-1.280177\S,0,-2.162051,-1.398159,-2.000995\N,0,-1.633055,-0.442933,-0.660482\Rh,0,0.637965,-0.090258,-0.108728\C,0,-2.711845,-0.038575,0.181827\C,0,-2.600673,-1.128025,0.935067\C,0,-3.425482,1.228403,0.217427\C,0,-4.289261,1.53115,1.293799\C,0,-3.282136,2.148662,-0.842715\C,0,-4.99775,2.735493,1.307964\H,0,-4.388464,0.820568,2.120035\C,0,-3.997891,3.351284,-0.82282\H,0,-2.620346,1.902558,-1.674767\C,0,-4.854749,3.649317,0.249046\H,0,-5.661489,2.966169,2.145956\H,0,-3.889392,4.057898,-1.650312\H,0,-5.410828,4.590952,0.260825\C,0,-2.590989,-2.542021,1.11097\C,0,-3.501534,-3.091924,2.239454\C,0,-2.012258,-3.189758,2.369614\H,0,-4.077474,-3.98429,1.979057\H,0,-4.036033,-2.366062,2.855729\H,0,-1.495619,-2.526953,3.064702\H,0,-1.544196,-4.168391,2.2262\O,0,-3.117944,-0.653521,-2.834581\O,0,-0.974284,-2.042167,-2.576091\\Version=ES64L-G09RevD.01\State=3-A\HF=-2278.070694\S2=2.011416\S2-1=0.\S2A=2.000064\RMSD=5.865e-09\Dipole=-0.9989291,-0.8638533,3.2844535\Quadrupole=-14.1448424,19.696611,-5.5517686,-6.1859341,-23.6738089,-14.1663524\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C⁻³TS4

1\1\GINB-A759\SP\UBPW91\GenECP\C20H23N1O11Rh2S1(3)\SIOC001\15-Mar-2018\0\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\\Title Card Required\\0,3\Rh,0,-2.922053,0.793867,-0.255091\Rh,0,-0.649251,-0.07771,0.114177\O,0,-2.133106,2.676162,-0.323035\C,0,-0.86791,2.838457,-0.158946\O,0,-0.013021,1.898348,0.014378\O,0,-2.60887,0.604252,-2.283311\C,0,-1.483672,0.148175,-2.696069\O,0,-0.485484,-0.21643,-1.969672\O,0,-3.604337,-1.133033,-0.167349\C,0,-2.771026,-2.089378,0.042163\O,0,-1.501166,-1.954532,0.166576\O,0,-3.143852,0.953969,1.780784\C,0,-2.147771,0.620154,2.524378\O,0,-1.013385,0.167203,2.13109\N,0,1.584188,-0.784825,0.425454\C,0,-0.354084,4.262613,-0.142447\C,0,-2.317283,0.802848,4.019583\C,0,-1.324697,-0.003279,-4.198323\C,0,-3.336117,-3.486273,0.179927\S,0,2.098858,-1.91168,1.714396\O,0,3.508451,-1.645135,2.08317\O,0,1.045331,-2.034907,2.720683\C,0,2.441688,-1.093156,-0.716561\C,0,3.017038,0.024325,-0.374125\C,0,3.648649,1.274943,-0.197352\C,0,3.622146,2.236312,-1.247062\C,0,4.337194,1.579281,1.01026\C,0,4.285486,3.455853,-1.09151\H,0,3.081367,2.007788,-2.168108\C,0,4.975022,2.812562,1.152611\H,0,4.351084,0.837434,1.810848\C,0,4.959097,3.752342,0.106177\H,0,4.269631,4.185032,-1.90649\H,0,5.496916,3.041958,2.085675\H,0,5.468531,4.712499,0.224222\C,0,2.59063,-2.415963,-1.34792\O,0,2.036315,-3.369815,0.859039\C,0,2.957322,-3.436001,-0.268596\H,0,2.86522,-4.466798,-0.643056\H,0,3.985239,-3.270019,0.097116\C,0,3.147133,-2.563356,-2.749606\H,0,3.797461,-3.421744,-2.94246\H,0,3.441568,-1.651557,-3.27557\C,0,1.678214,-2.812671,-2.499093\H,0,0.952771,-2.065734,-2.824959\H,0,1.316712,-3.844859,-2.504604\H,0,-2.610927,-4.229755,-0.17868\H,0,-3.529

775,-3.688741,1.246583\H,0,-4.284552,-3.573419,-0.36747\H,0,-1.520569,
-1.05135,-4.480686\H,0,-2.042934,0.638103,-4.726147\H,0,-0.297646,0.24
3157,-4.503992\H,0,-1.769633,0.018512,4.560242\H,0,-1.893744,1.777611,
4.314222\H,0,-3.381843,0.790055,4.289973\H,0,-0.972922,4.899973,-0.789
312\H,0,-0.419648,4.654123,0.886623\H,0,0.697943,4.29594,-0.455145\\Ve
rsion=ES64L-G09RevD.01\State=3-A\HF=-2278.0787215\S2=2.007319\S2-1=0.\
S2A=2.000034\RMSD=4.859e-09\Dipole=1.4876791,0.6581067,-2.753902\Quad
rupole=-9.2452966,11.9330125,-2.6877159,12.4871738,-13.7843391,13.34914
65\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-³INT4

1\1\GINB-A751\SP\UBPW91\GenECP\C20H23N1O11Rh2S1(3)\SIOC001\01-Mar-2018
\0\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\\Title C
ard Required\\0,3Rh,0,2.989889,0.60453,0.188644Rh,0,0.650492,-0.1314
21,-0.025451\O,0,2.3057,2.272533,1.193556\C,0,1.043493,2.389551,1.3991
49\O,0,0.11973,1.578598,1.019539\O,0,3.090428,-0.409953,1.964919\C,0,2
.065685,-1.052757,2.392427\O,0,0.926569,-1.118097,1.802236\O,0,3.54990
8,-1.097946,-0.825111\C,0,2.628681,-1.906816,-1.214986\O,0,1.364237,-1
.786422,-1.021667\O,0,2.805654,1.584436,-1.596769\C,0,1.677744,1.56661
1,-2.213497\O,0,0.618927,0.968328,-1.808642\N,0,-1.724321,-0.637066,-0
.357733\C,0,0.593989,3.597272,2.200381\C,0,1.586422,2.341643,-3.511981
\C,0,2.211104,-1.795447,3.705785\C,0,3.074386,-3.114595,-2.015414\S,0,
-2.468305,-1.580377,-1.838389\O,0,-3.87908,-1.170217,-2.045645\O,0,-1.
511109,-1.703363,-2.942174\C,0,-2.585587,-1.04139,0.790057\C,0,-2.7811
23,0.180313,0.352482\C,0,-3.311815,1.505553,0.265945\C,0,-2.837992,2.3
90844,-0.731375\C,0,-4.323368,1.931715,1.162249\C,0,-3.375013,3.678518
, -0.827306\H,0,-2.049033,2.057685,-1.408859\C,0,-4.842716,3.224326,1.0
61408\H,0,-4.69239,1.243846,1.927403\C,0,-4.37368,4.099863,0.065905\H,
0,-3.010628,4.359111,-1.601554\H,0,-5.6216,3.550654,1.755952\H,0,-4.78
8745,5.108381,-0.013129\C,0,-2.879551,-2.396718,1.242392\O,0,-2.452262
, -3.109069,-1.090944\C,0,-3.359142,-3.223981,0.04168\H,0,-3.375261,-4.
298158,0.28336\H,0,-4.36873,-2.905926,-0.268789\C,0,-3.440844,-2.67503
,2.62552\H,0,-4.177392,-3.479704,2.707802\H,0,-3.634369,-1.81903,3.276
657\C,0,-2.008985,-3.038776,2.318388\H,0,-1.203749,-2.428264,2.729852\
H,0,-1.757485,-4.092702,2.171966\H,0,2.405733,-3.965819,-1.826254\H,0,
3.016371,-2.872246,-3.089723\H,0,4.113674,-3.375339,-1.773266\H,0,2.01
2373,-2.867462,3.549136\H,0,3.221297,-1.664788,4.114536\H,0,1.469008,-
1.422585,4.429448\H,0,0.938651,1.811134,-4.224227\H,0,1.137846,3.32964
1,-3.314283\H,0,2.585944,2.493335,-3.940999\H,0,0.499577,3.311894,3.26
1674\H,0,1.335088,4.404452,2.124608\H,0,-0.389918,3.942642,1.85371\\Ve
rsion=ES64L-G09RevD.01\State=3-A\HF=-2278.0888761\S2=2.006199\S2-1=0.\
S2A=2.000024\RMSD=3.384e-09\Dipole=-1.8480616,0.3105259,3.0218419\Quad
rupole=-10.7585338,14.1487817,-3.3902479,-7.5536047,-20.243044,-14.268
116\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-³TS5

1\1\GINB-A761\SP\UBPW91\GenECP\C20H23N1O11Rh2S1(3)\SIOC001\15-Mar-2018
\0\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\Title C
ard Required\0,3\C,0,4.159195,2.209161,0.71402\H,0,4.866333,2.589689,
1.466424\H,0,3.947888,3.016578,-0.009197\O,0,4.849169,1.119851,0.04560
3\S,0,4.098365,0.70554,-1.426319\C,0,2.169548,0.835993,0.398596\Rh,0,-
0.642231,-0.010548,0.016125\C,0,1.443479,-0.349385,0.155887\N,0,2.3517
54,0.751611,-0.960886\C,0,1.961249,-1.719082,0.352984\C,0,2.954027,-1.
985559,1.326383\C,0,1.4847,-2.790756,-0.4375\C,0,3.44122,-3.284373,1.5
13018\H,0,3.355127,-1.16472,1.923938\C,0,1.987982,-4.083498,-0.260664\
H,0,0.737162,-2.584391,-1.203857\C,0,2.960664,-4.337357,0.719988\H,0,4
.210438,-3.471136,2.267825\H,0,1.623659,-4.898055,-0.893557\H,0,3.3505
93,-5.35001,0.857977\C,0,2.874261,1.68992,1.358748\C,0,2.81455,1.40515
3,2.857409\C,0,2.126651,2.627737,2.320328\O,0,4.587427,-0.647855,-1.72
5076\O,0,4.273895,1.813548,-2.383034\O,0,-3.34718,-1.600982,0.633926\C
,0,-2.295695,-2.238001,1.007935\O,0,-1.076864,-1.853408,0.878248\O,0,-
3.079834,1.07778,1.649513\C,0,-1.986551,1.211718,2.306973\O,0,-0.82223
3,0.850316,1.896398\O,0,-2.754019,2.087141,-1.0597\C,0,-1.543803,2.502
975,-1.184616\O,0,-0.479917,1.874156,-0.835109\O,0,-2.967952,-0.599274
, -2.05529\C,0,-1.818664,-0.954734,-2.508243\O,0,-0.702803,-0.843026,-1
.884462\C,0,-2.512242,-3.570814,1.696756\C,0,-1.782648,-1.589738,-3.88
114\C,0,-2.072753,1.869462,3.667351\C,0,-1.350059,3.882196,-1.780925\H
,0,-1.887058,2.951406,3.559943\H,0,-3.07634,1.734021,4.092587\H,0,-1.3
10786,1.457264,4.34329\H,0,-1.298535,4.624598,-0.966804\H,0,-0.406433,
3.924352,-2.342004\H,0,-2.198348,4.140161,-2.429332\H,0,-2.600777,-3.4
03555,2.783325\H,0,-3.443406,-4.035314,1.344392\H,0,-1.655549,-4.23564
7,1.522265\H,0,-0.794617,-1.452832,-4.340607\H,0,-1.976484,-2.671191,-
3.784069\H,0,-2.567939,-1.159969,-4.518415\Rh,0,-3.099771,0.252711,-0.
212307\H,0,2.583139,3.607882,2.491159\H,0,1.037918,2.62246,2.259123\H,
0,3.743997,1.526758,3.421522\H,0,2.185815,0.572314,3.181704\Version=E
S64L-G09RevD.01\State=3-A\HF=-2278.0792415\S2=2.00859\S2-1=0.\S2A=2.00
0039\RMSD=4.798e-09\Dipole=-2.3628253,0.4779152,3.2157218\Quadrupole=-
30.1373137,21.2993674,8.8379462,4.5917185,22.8182558,9.9936367\PG=C01
[X(C20H23N1O11Rh2S1)]\@

C-³INT5

1\1\GINB-A749\SP\UBPW91\GenECP\C20H23N1O11Rh2S1(3)\SIOC001\01-Mar-2018
\0\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\Title C
ard Required\0,3\C,0,-2.378385,-2.660598,1.099128\H,0,-2.521377,-3.44
5361,1.858059\H,0,-1.711766,-3.029975,0.307224\O,0,-3.70932,-2.453512,
0.564294\O,0,-5.166601,-1.681928,-1.272657\S,0,-3.764536,-1.580094,-0.
864151\O,0,-2.677803,-2.056803,-1.746548\N,0,-3.531263,0.0355,-0.43460
8\C,0,-2.455965,0.522468,0.177114\Rh,0,0.490382,-0.001264,0.145036\Rh,
0,2.827608,-0.177032,-0.598906\O,0,0.650945,-2.068701,0.434287\O,0,2.8
35569,-2.174685,-0.237854\O,0,1.266707,0.363275,2.051022\C,0,2.54278,0
.398696,2.219596\O,0,3.439811,0.206757,1.322377\O,0,0.611772,2.000082,

-0.23445\O,0,2.764646,1.819801,-0.960773\O,0,-0.055979,-0.301523,-1.80
0434\C,0,0.848365,-0.517112,-2.689214\O,0,2.118227,-0.540178,-2.487762
\C,0,0.353358,-0.743229,-4.099695\C,0,3.025372,0.692358,3.626132\C,0,-
1.437987,-0.275559,0.854206\C,0,1.741026,-2.698451,0.184013\C,0,1.7279
54,-4.19685,0.399677\C,0,1.696066,2.489624,-0.723376\C,0,1.697514,3.96
1272,-1.062607\C,0,-2.420001,2.012079,0.219207\C,0,-1.830925,2.685549,
1.309717\C,0,-3.071553,2.766292,-0.781632\C,0,-1.892799,4.081853,1.400
003\H,0,-1.328761,2.105092,2.088095\C,0,-3.1208,4.161375,-0.696521\H,0
, -3.538783,2.238124,-1.615556\C,0,-2.535597,4.82389,0.39644\H,0,-1.445
388,4.591119,2.25859\H,0,-3.623018,4.735454,-1.480461\H,0,-2.587269,5.
914377,0.468196\H,0,2.734334,-4.612014,0.260554\H,0,1.361062,-4.429003
,1.410871\H,0,1.036448,-4.663459,-0.320095\H,0,-0.589937,-1.306296,-4.
075838\H,0,0.154487,0.2324,-4.573826\H,0,1.112537,-1.272541,-4.690899\
H,0,2.685646,4.396029,-0.85562\H,0,1.493305,4.080072,-2.139835\H,0,0.9
13972,4.484968,-0.500064\H,0,2.693431,-0.108187,4.306325\H,0,4.120291,
0.762724,3.649906\H,0,2.581063,1.634026,3.983904\C,0,-1.825004,-1.3949
12,1.749183\C,0,-2.477171,-1.017509,3.093421\C,0,-1.090008,-1.593138,3
.074067\H,0,-3.315793,-1.638513,3.420544\H,0,-2.590506,0.046816,3.3124
81\H,0,-0.251078,-0.923932,3.267663\H,0,-0.942283,-2.624852,3.407392\
Version=ES64L-G09RevD.01\State=3-A\HF=-2278.1180495\S2=2.010586\S2-1=0
,\S2A=2.000052\RMSD=3.449e-09\Dipole=4.1788739,1.5681984,1.9656785\Qua
drupole=-42.077435,25.9599427,16.1174923,-10.9809068,-4.6172166,-9.282
7687\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C⁻³TS6

1\1\GINB-A738\SP\UBFW91\GenECP\C20H23N1O11Rh2S1(3)\SIOC001\28-Feb-2018
\0\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\Title C
ard Required\0,3\C,0,-2.202287,-3.246863,0.765289\H,0,-2.461432,-4.14
1496,1.351722\H,0,-1.346096,-3.484648,0.111712\O,0,-3.380534,-2.945699
, -0.036962\S,0,-3.032865,-2.012929,-1.41785\C,0,-1.855392,-0.852994,0.
825555\Rh,0,0.589439,-0.060772,-0.021463\N,0,-1.834854,-0.745483,-0.66
5204\C,0,-2.487307,0.193023,0.293815\C,0,-3.205114,1.420936,0.23487\C,
0,-3.564811,2.100919,1.428557\C,0,-3.575929,1.96897,-1.019573\C,0,-4.2
71978,3.302399,1.360637\H,0,-3.274999,1.681249,2.395076\C,0,-4.29398,3
.166017,-1.070933\H,0,-3.304349,1.437975,-1.933551\C,0,-4.642065,3.837
832,0.113516\H,0,-4.541912,3.824465,2.282711\H,0,-4.58459,3.579495,-2.
040414\H,0,-5.202461,4.775508,0.066478\C,0,-1.893193,-2.055417,1.66509
3\C,0,-2.49819,-1.966475,3.063808\C,0,-1.02824,-2.244381,2.905572\H,0,
-3.16512,-2.780223,3.362362\H,0,-2.804202,-0.978341,3.415566\H,0,-0.31
3617,-1.449204,3.119155\H,0,-0.661834,-3.257715,3.091833\O,0,-4.333123
, -1.43214,-1.801832\O,0,-2.227249,-2.80728,-2.360104\O,0,2.348064,2.46
8718,-0.783018\C,0,1.089668,2.678388,-0.926714\O,0,0.136808,1.849685,-
0.681586\O,0,2.810196,1.276869,1.824196\C,0,1.689785,1.163349,2.434387
\O,0,0.62227,0.632394,1.950932\O,0,3.458262,-1.274004,0.549329\C,0,2.5
20697,-2.129988,0.729673\O,0,1.2551,-1.931299,0.599063\O,0,3.060763,-0

.04552,-2.038167\C,0,1.997283,-0.536471,-2.570304\O,0,0.862284,-0.6669
4,-1.988997\C,0,0.682758,4.033942,-1.471616\C,0,2.082982,-0.972373,-4.
017537\C,0,1.605172,1.729157,3.837546\C,0,2.947963,-3.536133,1.107604\
H,0,2.606505,1.8003,4.282814\H,0,1.170841,2.741891,3.790803\H,0,0.9496
34,1.110457,4.466836\H,0,2.979168,-4.158143,0.197349\H,0,3.95072,-3.52
4908,1.555258\H,0,2.22419,-3.988807,1.799945\H,0,1.386627,4.807346,-1.
133726\H,0,0.716023,4.002159,-2.573626\H,0,-0.34188,4.281712,-1.163734
\H,0,3.116377,-1.24033,-4.276631\H,0,1.404138,-1.816427,-4.201383\H,0,
1.768812,-0.135702,-4.663828\Rh,0,2.957441,0.616713,-0.11096\\Version=
ES64L-G09RevD.01\State=3-A\HF=-2278.0823576\S2=2.007028\S2-1=0.\S2A=2.
000032\RMSD=7.762e-09\Dipole=0.1899045,0.9155636,2.8911244\Quadrupole=
-26.1103009,14.9125642,11.1977367,-20.6738628,-14.2794162,-12.1362227\
PG=C01 [X(C20H23N1O11Rh2S1)]\ \@

C-³INT6

1\1\GINB-A744\SP\UBPW91\GenECP\C20H23N1O11Rh2S1(3)\SIOC001\01-Mar-2018
\0\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\\Title C
ard Required\0,3\Rh,0,-0.615182,0.173266,-0.019292\Rh,0,-2.791212,-0.
99016,0.090615\O,0,-1.579879,1.693776,-1.011415\C,0,-2.83719,1.589359,
-1.245057\O,0,-3.586837,0.626879,-0.834954\O,0,-1.106469,1.027022,1.81
4901\C,0,-2.222092,0.710007,2.374301\O,0,-3.120138,-0.078317,1.903836\
O,0,0.163207,-1.430005,0.988948\C,0,-0.572598,-2.447901,1.249094\O,0,-
1.841974,-2.505159,1.030865\O,0,-0.353745,-0.744852,-1.837231\C,0,-1.2
42996,-1.55963,-2.274978\O,0,-2.366056,-1.847473,-1.70828\C,0,-3.48604
3,2.677328,-2.067578\C,0,-0.923096,-2.267297,-3.572221\C,0,-2.488646,1
.309741,3.739896\C,0,0.102057,-3.640663,1.876863\C,0,3.590165,1.675078
,1.878287\C,0,2.989211,0.462552,2.521596\C,0,3.459461,0.396629,1.05789
9\C,0,2.394356,0.181771,0.009464\N,0,2.404962,-0.861047,-0.805273\S,0,
3.545012,-2.083455,-0.719267\O,0,4.443943,-1.793479,0.674436\C,0,4.737
628,-0.37618,0.791239\O,0,2.858972,-3.356463,-0.443454\O,0,4.429301,-1
.959884,-1.891394\C,0,1.240348,1.071002,-0.058758\C,0,1.384262,2.49006
8,-0.310712\C,0,2.459414,2.961258,-1.126344\C,0,2.626976,4.323337,-1.3
85428\C,0,1.733973,5.264654,-0.843949\C,0,0.667229,4.824047,-0.040599\
C,0,0.485286,3.463341,0.217094\H,0,2.94108,2.51732,1.640313\H,0,4.6114
93,1.958276,2.151946\H,0,3.571368,-0.110393,3.249346\H,0,1.908766,0.45
1523,2.680143\H,0,5.439567,-0.295043,1.634674\H,0,5.247517,-0.024489,-
0.12442\H,0,3.144521,2.232746,-1.567891\H,0,3.45533,4.65453,-2.018755\
H,0,1.867865,6.330955,-1.046514\H,0,-0.025806,5.552038,0.392265\H,0,-0
.33154,3.129177,0.857751\H,0,-0.588583,-4.492354,1.925958\H,0,0.997186
, -3.893986,1.287963\H,0,0.435874,-3.380634,2.894555\H,0,-1.8401,-2.649
108,-4.040268\H,0,-0.390038,-1.589037,-4.253014\H,0,-0.252312,-3.11499
5,-3.354659\H,0,-2.053155,0.652102,4.510759\H,0,-2.014969,2.29716,3.82
7212\H,0,-3.569728,1.382003,3.920215\H,0,-2.938873,3.622522,-1.952681\
H,0,-3.452332,2.387029,-3.131169\H,0,-4.53917,2.798105,-1.778788\\Vers
ion=ES64L-G09RevD.01\State=3-A\HF=-2278.1291255\S2=2.009345\S2-1=0.\S2

A=2.000052\RMSD=3.381e-09\Dipole=-2.269656,3.0478156,1.8395687\Quadrupole=-8.2376205,-0.9225065,9.160127,12.2590377,14.4951015,-5.0007503\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-³TS7

1\1\GINB-A751\SP\UBPW91\GenECP\C20H23N1O11Rh2S1(3)\SIOC001\28-Feb-2018\0\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\Title Card Required\0,3\O,0,-2.955966,-2.608826,0.732435\O,0,-5.016719,-2.422453,-0.70514\S,0,-3.589948,-2.131996,-0.847258\O,0,-2.764839,-2.79805,-1.864591\N,0,-3.388036,-0.492049,-0.858674\C,0,-2.602515,0.19578,-0.049159\Rh,0,0.434518,0.07274,0.027181\Rh,0,2.829989,0.009999,-0.419536\O,0,0.199599,-1.308912,-1.50106\O,0,2.455391,-1.383314,-1.884958\O,0,1.137429,-1.81566,1.492068\C,0,2.373225,-2.080469,1.542549\O,0,3.301506,-1.465859,0.881563\O,0,0.884253,1.431967,1.5805\O,0,3.117452,1.406389,1.058453\O,0,0.446962,1.800078,-1.450755\C,0,1.539799,2.080167,-2.029232\O,0,2.667654,1.492025,-1.792957\C,0,1.551667,3.166262,-3.088984\C,0,2.856227,-3.222199,2.42715\C,0,-1.495491,-0.317814,0.810689\C,0,-1.658696,-2.213393,0.874048\C,0,1.244597,-1.735266,-2.120944\C,0,1.017415,-2.721696,-3.246867\C,0,2.101755,1.813859,1.728638\C,0,2.370883,2.87769,2.777294\C,0,-2.84736,1.663379,-0.030768\C,0,-2.064446,2.542247,0.752022\C,0,-3.940643,2.187413,-0.762573\C,0,-2.378096,3.906092,0.807554\H,0,-1.190328,2.175656,1.293844\C,0,-4.23929,3.550303,-0.710816\H,0,-4.550283,1.505772,-1.358065\C,0,-3.461848,4.415886,0.078006\H,0,-1.761746,4.57429,1.415249\H,0,-5.086938,3.939492,-1.281463\H,0,-3.701099,5.4823,0.121549\H,0,0.026395,-3.185154,-3.15794\H,0,1.069676,-2.185321,-4.209097\H,0,1.808201,-3.485748,-3.247086\H,0,0.989123,2.817064,-3.970114\H,0,1.040675,4.063285,-2.707876\H,0,2.577937,3.414781,-3.390109\H,0,2.322924,3.87173,2.301523\H,0,1.614708,2.840949,3.573692\H,0,3.377693,2.752748,3.19934\H,0,2.379931,-3.161113,3.417412\H,0,2.558933,-4.182253,1.973532\H,0,3.948902,-3.205337,2.535123\C,0,-1.710465,-0.589464,2.150556\C,0,-2.669308,-0.6082,3.270896\C,0,-1.147258,-0.74848,3.495757\H,0,-3.27904,-1.507778,3.411813\H,0,-3.187946,0.326478,3.512304\H,0,-0.564608,0.096192,3.87693\H,0,-0.773311,-1.725193,3.817575\H,0,-1.155245,-2.70741,1.710551\H,0,-1.034638,-2.274045,-0.035218\Version=ES64L-G09RevD.01\State=3-A\HF=-2278.0577517\S2=2.006671\S2-1=0.\S2A=2.000026\RMSD=3.667e-09\Dipole=0.06414,1.6806158,3.0034864\Quadrupole=-29.0487529,13.3150725,15.7336804,-17.6433741,-7.5307791,-6.2374981\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-³TS9

1\1\GINB-A751\SP\UBPW91\GenECP\C20H23N1O11Rh2S1(3)\SIOC001\28-Feb-2018\0\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\Title Card Required\0,3\C,0,-3.129512,2.58859,-0.683421\O,0,-2.364921,2.478241,0.541126\S,0,-0.687801,2.624263,0.396366\O,0,-0.229316,2.80315,1.778529\O,0,-0.414769,3.657684,-0.629912\Rh,0,1.432074,0.093991,-0.000949\O,0,1.215627,-0.204519,2.020231\C,0,2.104105,-0.873833,2.662681\C,0,1

.899926,-1.002829,4.155402\O,0,2.572141,1.765961,0.36824\C,0,3.837193,
1.632123,0.554038\C,0,4.604247,2.898112,0.865317\Rh,0,3.457609,-1.1923
35,0.148573\O,0,3.147213,-1.423396,2.150188\O,0,1.811958,0.280848,-2.0
22266\C,0,2.868756,-0.262859,-2.51364\C,0,3.085248,-0.093783,-4.001651
\O,0,0.424291,-1.6681,-0.37776\C,0,1.095494,-2.766719,-0.405823\C,0,0.
310028,-4.029236,-0.691106\O,0,4.495191,0.528659,0.516659\O,0,3.742026
, -0.936757,-1.856812\O,0,2.359679,-2.88391,-0.222998\H,0,-2.561624,3.1
86229,-1.4132\H,0,-4.041582,3.138648,-0.409115\C,0,-2.374295,0.25958,-
1.591244\H,0,4.272614,3.710804,0.202941\H,0,4.385545,3.205793,1.900993
\H,0,5.683839,2.729475,0.759212\H,0,2.589811,-1.746638,4.574747\H,0,2.
083897,-0.025295,4.630016\H,0,0.857518,-1.281046,4.36947\H,0,4.06894,-
0.484397,-4.292333\H,0,2.29847,-0.63549,-4.55097\H,0,3.003834,0.96994,
-4.271703\H,0,0.951701,-4.912596,-0.57913\H,0,-0.549553,-4.097582,-0.0
07084\H,0,-0.08573,-3.99248,-1.718857\C,0,-3.498693,1.209114,-1.258856
\C,0,-3.011937,0.929093,-2.730916\C,0,-4.731331,0.624529,-0.820022\C,0
, -5.775006,0.105039,-0.42843\C,0,-6.987289,-0.482044,0.030915\C,0,-7.5
01535,-1.657999,-0.574546\C,0,-7.702893,0.099881,1.109544\C,0,-8.69139
8,-2.22853,-0.111852\H,0,-6.954845,-2.110919,-1.405238\C,0,-8.892072,-
0.479059,1.56256\H,0,-7.309519,1.003473,1.581055\C,0,-9.391387,-1.6434
63,0.956117\H,0,-9.075608,-3.13548,-0.587333\H,0,-9.432652,-0.020104,2
.395103\H,0,-10.321443,-2.09344,1.314176\H,0,-2.44391,-0.813722,-1.397
307\H,0,-2.530739,1.797288,-3.195592\H,0,-3.656849,0.355578,-3.406684\
H,0,-1.098499,0.730764,-0.883132\N,0,-0.277628,1.117332,-0.175311\\Ver
sion=ES64L-G09RevD.01\State=3-A\HF=-2278.0701375\S2=2.006159\S2-1=0.\S
2A=2.000023\RMSD=3.238e-09\Dipole=-0.3442451,-2.4832915,-1.5371949\Qua
drupole=12.0000165,-15.6585684,3.6585519,12.8941232,1.5653692,-1.97317
08\PG=C01 [X(C20H23N1O11Rh2S1)]\@

C-³INT7

1\1\GINB-A753\SP\UBPW91\GenECP\C20H23N1O11Rh2S1(3)\SIOC001\01-Mar-2018
\0\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\\Title C
ard Required\\0,3\C,0,3.195481,2.898401,-0.107575\O,0,2.466207,2.17487
6,-1.12572\S,0,0.781785,2.295705,-1.107556\O,0,0.382249,1.930188,-2.46
7592\O,0,0.441383,3.620615,-0.535667\N,0,0.36703,1.071589,-0.056494\Rh
,0,-1.372309,0.034318,-0.011812\O,0,-1.102956,-0.893232,-1.822786\C,0,
-2.00589,-1.697317,-2.255908\C,0,-1.737232,-2.357314,-3.589503\O,0,-2.
407854,1.552316,-0.929895\C,0,-3.671028,1.42565,-1.125162\C,0,-4.35506
1,2.554166,-1.862898\Rh,0,-3.459923,-1.139226,0.163949\O,0,-3.101825,-
1.994284,-1.650953\O,0,-1.775235,0.857178,1.838641\C,0,-2.879758,0.556
443,2.425895\C,0,-3.154174,1.241902,3.746584\O,0,-0.481611,-1.567069,0
.942632\C,0,-1.214793,-2.565005,1.289515\C,0,-0.521835,-3.693434,2.022
246\O,0,-4.390347,0.422931,-0.76647\O,0,-3.774391,-0.248915,1.979801\O
,0,-2.477766,-2.677426,1.087626\H,0,2.56537,3.706392,0.295239\H,0,0.83
0281,1.236837,0.857722\H,0,4.060048,3.33854,-0.628156\C,0,2.720022,1.5
50831,2.087472\H,0,-3.962204,3.522015,-1.520251\H,0,-4.130781,2.4663,-

2.93871\H,0,-5.442306,2.503222,-1.718453\H,0,-2.630869,-2.888254,-3.94
2261\H,0,-1.426012,-1.599052,-4.323246\H,0,-0.90584,-3.072513,-3.48095
1\H,0,-3.579795,2.240099,3.550306\H,0,-3.877671,0.662118,4.335155\H,0,
-2.219594,1.379148,4.308344\H,0,-1.123538,-4.610383,1.96852\H,0,0.4784
74,-3.863386,1.59924\H,0,-0.397627,-3.414324,3.08184\C,0,3.679571,1.97
587,1.017911\C,0,3.657246,2.610418,2.458127\C,0,4.73969,1.063701,0.687
649\C,0,5.636259,0.276282,0.395486\C,0,6.685986,-0.617948,0.038799\C,0
,7.503756,-1.212734,1.033422\C,0,6.934723,-0.924855,-1.323869\C,0,8.53
5441,-2.085071,0.671907\H,0,7.317444,-0.978948,2.084521\C,0,7.970135,-
1.797451,-1.673303\H,0,6.305551,-0.470786,-2.093\C,0,8.774032,-2.38058
6,-0.680142\H,0,9.158587,-2.535867,1.4496\H,0,8.150901,-2.024575,-2.72
7786\H,0,9.582763,-3.061951,-0.958515\H,0,2.636858,0.550485,2.516772\H
,0,3.320889,3.654742,2.469477\H,0,4.483448,2.399482,3.1479\\Version=ES
64L-G09RevD.01\State=3-A\HF=-2278.0746426\S2=2.005667\S2-1=0.\S2A=2.00
002\RMSD=4.942e-09\Dipole=-0.2087964,-1.5033743,2.2299444\Quadrupole=5
.3785142,-7.8876483,2.5091341,-10.1620941,7.4314545,10.1282837\PG=C01
[X(C20H23N1O11Rh2S1)]\@

C-³TS10

1\1\GINB-A759\SP\UBPW91\GenECP\C20H23N1O11Rh2S1(3)\SIOC001\15-Mar-2018
\0\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\\Title C
ard Required\\0,3\C,0,3.334698,2.143686,0.618055\O,0,2.447316,2.433221
, -0.483336\S,0,0.797961,2.33611,-0.159788\O,0,0.214683,3.107472,-1.270
586\O,0,0.567081,2.710691,1.247403\N,0,0.502378,0.667288,-0.296541\Rh,
0,-1.500966,0.002679,-0.117451\O,0,-1.818287,0.25772,-2.127784\C,0,-2.
962947,-0.042591,-2.629572\C,0,-3.155538,0.227276,-4.103774\O,0,-2.300
952,1.854157,0.267024\C,0,-3.56591,1.977222,0.444465\C,0,-4.069171,3.3
69083,0.755183\Rh,0,-3.753435,-0.86889,0.025882\O,0,-3.955024,-0.53158
7,-1.974493\O,0,-1.335943,-0.345036,1.906107\C,0,-2.335993,-0.83604,2.
542143\C,0,-2.176186,-1.032752,4.032457\O,0,-0.856484,-1.932108,-0.516
005\C,0,-1.733168,-2.871389,-0.546347\C,0,-1.219551,-4.273752,-0.79783
\O,0,-4.432611,1.027072,0.40048\O,0,-3.467322,-1.156878,2.01764\O,0,-2
.997496,-2.736012,-0.360712\H,0,2.910046,2.560229,1.544173\H,0,4.25838
7,2.685995,0.371942\C,0,2.563164,-0.356141,0.487161\H,0,-5.155401,3.42
7595,0.606349\H,0,-3.836424,3.609059,1.805698\H,0,-3.549488,4.104384,0
.124537\H,0,-3.272698,1.312588,-4.25759\H,0,-2.266234,-0.09247,-4.6661
43\H,0,-4.050825,-0.287893,-4.47536\H,0,-2.97357,-1.678171,4.423397\H,
0,-1.189324,-1.465747,4.251415\H,0,-2.227988,-0.052102,4.533281\H,0,-0
.396345,-4.252987,-1.525993\H,0,-0.825522,-4.68778,0.14523\H,0,-2.0313
, -4.921974,-1.153592\C,0,3.647417,0.634702,0.771968\C,0,2.861145,-0.14
4002,1.89549\C,0,4.999572,0.241099,0.494201\C,0,6.15691,-0.082459,0.23
0637\C,0,7.502833,-0.442577,-0.058392\C,0,7.987749,-1.743017,0.238751\
C,0,8.390214,0.496221,-0.647308\C,0,9.313435,-2.086177,-0.044301\H,0,7
.310737,-2.47096,0.692401\C,0,9.713953,0.141939,-0.924943\H,0,8.023289
,1.498859,-0.879666\C,0,10.182315,-1.148063,-0.625683\H,0,9.672336,-3.

092321,0.190847\H,0,10.385194,0.877111,-1.378061\H,0,11.218497,-1.4206
16,-0.844297\H,0,2.646151,-1.267154,-0.105167\H,0,2.197928,0.504824,2.
481887\H,0,3.382753,-0.913271,2.480001\H,0,0.804506,0.41024,-1.252337\
\Version=ES64L-G09RevD.01\State=3-A\HF=-2278.0615374\S2=2.010774\S2-1=
0.\S2A=2.000049\RMSD=7.210e-09\Dipole=-1.0433457,-2.5165124,0.3554447\
Quadrupole=5.2534026,-8.0674692,2.8140666,-9.291747,0.9057098,1.466080
3\PG=C01 [X(C20H23N1O11Rh2S1)]\@

B-INT1

1\1\GINB-A748\SP\RBPW91\GenECP\C21H25N1O11Rh2S1\SI0C001\14-Mar-2018\0\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\Title Card
Required\0,1\Rh,0,-2.18301,-1.69096,0.334591\Rh,0,-1.571816,0.611909
, -0.078359\O,0,-3.530436,-1.056548,1.73125\C,0,-3.643479,0.204425,1.94
3423\O,0,-2.958243,1.12866,1.367682\O,0,-3.623237,-1.578647,-1.102378\
C,0,-3.774946,-0.454234,-1.703986\O,0,-3.093023,0.613975,-1.491998\O,0
, -0.82977,-2.287284,-1.06891\C,0,-0.158774,-1.378248,-1.678856\O,0,-0.
259995,-0.110431,-1.484066\O,0,-0.735259,-1.77762,1.770669\C,0,-0.0328
92,-0.732042,1.999638\O,0,-0.15566,0.401093,1.396715\N,0,-1.232869,2.4
26276,-0.557337\C,0,-4.683555,0.662421,2.941146\C,0,1.037925,-0.810867
, 3.062717\C,0,-4.844435,-0.362424,-2.769861\C,0,0.857687,-1.824528,-2.
702654\S,0,0.202774,3.129632,-0.985961\O,0,0.220019,3.137009,-2.46551\
O,0,0.280099,4.396439,-0.216089\O,0,1.551702,2.210344,-0.587611\C,0,2.
247226,2.529878,0.647333\H,0,2.182468,3.613133,0.831341\H,0,1.770958,1
.98759,1.478367\C,0,3.896995,0.673746,0.341896\C,0,4.13388,-0.523454,0
.207753\C,0,4.410531,-1.909488,-0.004215\C,0,4.786242,-2.374431,-1.291
229\C,0,4.32171,-2.847855,1.054531\C,0,5.052286,-3.731501,-1.506797\H,
0,4.868863,-1.655546,-2.110154\C,0,4.588566,-4.202908,0.828744\H,0,4.0
45237,-2.499727,2.052615\C,0,4.952472,-4.651542,-0.450868\H,0,5.340656
, -4.07263,-2.505245\H,0,4.512789,-4.913001,1.657184\H,0,5.159269,-5.71
1283,-0.62341\H,0,0.500717,-2.729468,-3.214209\H,0,1.053632,-1.019668,
-3.423259\H,0,1.800172,-2.070004,-2.186513\H,0,1.033257,-1.801932,3.53
4088\H,0,2.019591,-0.617678,2.601609\H,0,0.866,-0.033764,3.823867\H,0,
-5.004413,-0.177243,3.571532\H,0,-4.282278,1.478431,3.559183\H,0,-5.55
6965,1.056122,2.395614\H,0,-5.486581,0.51045,-2.57858\H,0,-4.368139,-0
.21128,-3.751708\H,0,-5.44581,-1.280433,-2.789217\C,0,3.722201,2.11264
, 0.501284\C,0,4.564359,2.793723,1.654548\C,0,4.499498,3.032312,-0.5164
32\C,0,4.966934,3.92346,0.667218\H,0,5.414993,2.158597,1.942202\H,0,4.
005272,3.071705,2.563466\H,0,5.330849,2.484628,-0.983726\H,0,3.883949,
3.489586,-1.30502\H,0,6.025338,4.224137,0.671643\H,0,4.350878,4.828125
, 0.784583\Version=ES64L-G09RevD.01\State=1-A\HF=-2317.4089631\RMSD=4.
085e-09\Dipole=-0.1414569,-3.1883644,1.913769\Quadrupole=17.1448497,-2
4.3937623,7.2489126,0.4666259,1.1692082,14.8677796\PG=C01 [X(C21H25N1O
11Rh2S1)]\@

B-ITS2

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1\1\GINB-A757\SP\RBPW91\GenECP\C21H25N1O11Rh2S1\SIOC001\14-Mar-2018\0\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\Title Card
Required\0,1\O,0,-2.49999997,-0.68527918,0.\C,0,-3.32363097,-1.23178
718,-0.819251\O,0,-4.56986097,-1.46208918,-0.60317\O,0,-3.74821297,1.7
1093282,0.980117\C,0,-4.90382197,1.82266082,0.435684\O,0,-5.80966797,0
.90836582,0.406127\O,0,-4.01260997,0.50291882,3.614662\C,0,-5.24317097
,0.23977182,3.863909\O,0,-6.07962097,-0.32202118,3.065058\O,0,-2.72191
997,-1.87616718,2.623364\C,0,-3.59826697,-2.81319118,2.5718\O,0,-4.774
04597,-2.72075418,2.065412\C,0,-2.80240097,-1.63791918,-2.180401\C,0,-
3.21986397,-4.16069018,3.148869\C,0,-5.23756897,3.12458682,-0.254932\C
,0,-5.75486197,0.59464282,5.244938\H,0,-6.27899597,3.40797182,-0.04889
3\H,0,-4.54753397,3.91434782,0.070283\H,0,-5.13694897,2.98711882,-1.34
4363\H,0,-5.22975397,1.48090782,5.627251\H,0,-6.83925197,0.76601882,5.
224713\H,0,-5.55066097,-0.24599118,5.929054\H,0,-3.15612097,-2.6492781
8,-2.42826\H,0,-3.20634297,-0.95180018,-2.942498\H,0,-1.70555297,-1.59
642518,-2.198735\H,0,-2.23244097,-4.10987218,3.625599\H,0,-3.97749797,
-4.48043918,3.880497\H,0,-3.20391897,-4.91073818,2.342206\Rh,0,-3.2308
2797,-0.07838918,1.813002\C,0,-9.35032797,-3.45877018,0.845116\H,0,-10
.07426397,-4.26813118,0.657458\H,0,-8.41433697,-3.90168318,1.216654\O,
0,-9.13731297,-2.81619818,-0.427635\S,0,-7.55504997,-2.28774618,-0.694
553\N,0,-7.10703797,-1.81550418,0.846201\Rh,0,-5.41006997,-0.93380618,
1.199464\C,0,-9.92689897,-2.45058618,1.875241\C,0,-11.50822797,-2.4823
6718,1.925052\C,0,-9.93907997,-3.06060918,3.325641\O,0,-7.72626397,-1.
25937818,-1.738147\O,0,-6.73919897,-3.49950318,-0.967908\C,0,-9.371828
97,-1.11415718,1.677563\C,0,-9.28138597,0.11094782,1.527748\C,0,-9.224
09797,1.51167382,1.318812\C,0,-9.07966097,2.40731682,2.411537\C,0,-9.3
7352197,2.04211282,0.008868\C,0,-9.09174997,3.78866982,2.198198\H,0,-8
.96892897,2.00038382,3.419096\C,0,-9.38320097,3.42543782,-0.190851\H,0
,-9.46710597,1.35141782,-0.831628\C,0,-9.24584097,4.30343782,0.899309\
H,0,-8.98508197,4.46923782,3.047693\H,0,-9.50180297,3.82342982,-1.2025
86\H,0,-9.26101697,5.38496282,0.737556\C,0,-11.42340397,-3.47290918,3.
11832\H,0,-12.11292897,-3.29729018,3.957791\H,0,-12.00977097,-2.807408
18,1.000068\H,0,-11.91413697,-1.50522118,2.22562\H,0,-11.52426497,-4.5
2332618,2.801976\H,0,-9.20111497,-3.85542518,3.520515\H,0,-9.82144997,
-2.27457618,4.085976\Version=ES64L-G09RevD.01\State=1-A\HF=-2317.4025
153\RMSD=4.669e-09\Dipole=-0.1904745,1.5949855,2.6952431\Quadrupole=-5
.1834309,11.2523104,-6.0688795,-6.4630211,-14.3378171,-12.9490781\PG=C
01 [X(C21H25N1O11Rh2S1)]\@

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B-INT2

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1\1\GINB-A749\SP\RBPW91\GenECP\C21H25N1O11Rh2S1\SIOC001\14-Mar-2018\0\
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Required\0,1\Rh,0,-3.008517,0.338727,-0.396226\Rh,0,-0.669747,-0.075
698,0.060408\O,0,-2.449947,1.81862,-1.70588\C,0,-1.198961,2.039861,-1.

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877322\O,0,-0.227633,1.43461,-1.288097\O,0,-2.915046,-1.027505,-1.9202
22\C,0,-1.795426,-1.603785,-2.156222\O,0,-0.69042,-1.423175,-1.519795\
O,0,-3.487757,-1.153877,0.922457\C,0,-2.528123,-1.786706,1.495233\O,0,
-1.270789,-1.581418,1.327367\O,0,-3.019103,1.682568,1.154779\C,0,-1.92
8209,1.887355,1.795129\O,0,-0.794217,1.31942,1.571371\N,0,1.47747,-0.3
30999,0.455297\C,0,-0.815371,3.103149,-2.889147\C,0,-1.960879,2.913988
,2.910438\C,0,-1.761515,-2.599481,-3.301453\C,0,-2.907466,-2.866127,2.
489245\S,0,2.110172,-0.856597,2.196832\O,0,3.408,-0.182109,2.434522\O,
0,1.056689,-0.92537,3.210757\C,0,2.503766,-0.852313,-0.476145\C,0,2.54
0123,0.445657,-0.262135\C,0,2.989437,1.80336,-0.332868\C,0,2.343494,2.
799234,0.437077\C,0,4.098303,2.146709,-1.144142\C,0,2.811942,4.116191,
0.39658\H,0,1.480971,2.525958,1.048526\C,0,4.548501,3.468637,-1.182425
\H,0,4.597919,1.374089,-1.734306\C,0,3.909964,4.455242,-0.410796\H,0,2
.31608,4.883837,0.996726\H,0,5.404406,3.731575,-1.809846\H,0,4.270344,
5.487232,-0.438877\C,0,3.026315,-2.22223,-0.63286\O,0,2.407658,-2.470
819,1.771365\C,0,3.469791,-2.64912,0.792675\H,0,3.701123,-3.725612,0.8
25027\H,0,4.360043,-2.078494,1.106496\C,0,4.135606,-2.490952,-1.70297\
C,0,2.127617,-3.290188,-1.35265\H,0,-2.216007,-3.7171,2.408628\H,0,-2.
820332,-2.461711,3.511265\H,0,-3.942719,-3.193825,2.324749\H,0,-1.4663
35,-3.592017,-2.925705\H,0,-2.746741,-2.666869,-3.780611\H,0,-1.010599
, -2.288978,-4.045386\H,0,-1.321657,2.590322,3.744298\H,0,-1.570925,3.8
75269,2.535547\H,0,-2.991884,3.0685,3.255781\H,0,-0.449435,2.617039,-3
.808842\H,0,-1.683855,3.726622,-3.139531\H,0,0.001336,3.725526,-2.4950
53\C,0,3.387828,-3.791935,-2.11387\H,0,1.383905,-2.810883,-2.002267\H,
0,1.607085,-3.993916,-0.686104\H,0,3.273467,-3.972101,-3.192984\H,0,3.
832205,-4.691467,-1.659608\H,0,4.122402,-1.728489,-2.496762\H,0,5.1661
2,-2.585119,-1.322963\\Version=ES64L-G09RevD.01\State=1-A\HF=-2317.449
5572\RMSD=2.953e-09\Dipole=2.9100847,-0.1455572,-2.5302906\Quadrupole=
-5.9169228,16.94855,-11.0316271,-0.2486305,-18.8584724,6.3399387\PG=C0
1 [X(C21H25N1O11Rh2S1)]\@

B-¹TS3

1\1\GINB-A757\SP\RBPW91\GenECP\C21H25N1O11Rh2S1\SI0C001\17-Mar-2018\0\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\\Title Card
Required\\0,1\C,0,-3.349636,-2.761218,-0.054299\H,0,-3.912759,-3.6275
76,0.326038\H,0,-2.624449,-3.115828,-0.807085\O,0,-4.332402,-1.889111,
-0.668819\S,0,-3.65958,-0.850787,-1.850416\C,0,-2.239138,-0.722919,0.4
80584\Rh,0,0.778113,-0.023564,-0.060911\N,0,-2.106277,-0.318402,-0.967
4\C,0,-2.404514,0.559096,0.230403\C,0,-2.691038,1.941149,0.468965\C,0,
-2.871188,2.420591,1.790451\C,0,-2.799891,2.836305,-0.621705\C,0,-3.15
2497,3.771059,2.008869\H,0,-2.782768,1.729259,2.632192\C,0,-3.093561,4
.183229,-0.389964\H,0,-2.666322,2.457687,-1.636554\C,0,-3.267734,4.655
2,0.92148\H,0,-3.289227,4.137459,3.030021\H,0,-3.187717,4.868674,-1.23
6452\H,0,-3.496505,5.709909,1.097789\C,0,-2.621938,-2.014387,1.08799\C

, 0, -3.435607, -1.948564, 2.425492\C, 0, -1.584226, -2.933762, 1.829781\O, 0, -4.665973, 0.218025, -1.994498\O, 0, -3.20591, -1.650707, -3.001108\O, 0, 3.05712, 2.073821, 0.322932\C, 0, 1.892914, 2.598472, 0.473626\O, 0, 0.767649, 1.985928, 0.369762\O, 0, 3.178259, -0.333065, 1.919392\C, 0, 2.052914, -0.510829, 2.510529\O, 0, 0.889892, -0.45031, 1.962085\O, 0, 3.213472, -1.931152, -0.51548\C, 0, 2.092171, -2.546122, -0.645917\O, 0, 0.923731, -2.029563, -0.502632\O, 0, 3.099512, 0.481768, -2.091427\C, 0, 1.941194, 0.578926, -2.6454\O, 0, 0.808738, 0.418888, -2.062191\C, 0, 1.844587, 4.067739, 0.836871\C, 0, 1.908801, 0.9425, -4.114417\C, 0, 2.09742, -0.849002, 3.987183\C, 0, 2.147733, -4.018999, -0.995978\H, 0, 3.071538, -0.576444, 4.414196\H, 0, 1.287977, -0.331028, 4.521925\H, 0, 1.94747, -1.93381, 4.117569\H, 0, 1.534223, -4.210535, -1.889787\H, 0, 3.183407, -4.33344, -1.178205\H, 0, 1.724691, -4.613669, -0.17048\H, 0, 1.893678, 4.169946, 1.934044\H, 0, 2.707221, 4.59535, 0.406834\H, 0, 0.904086, 4.517488, 0.491368\H, 0, 2.827976, 0.605291, -4.612785\H, 0, 1.024065, 0.502958, -4.595252\H, 0, 1.844398, 2.039125, -4.213746\Rh, 0, 3.169479, 0.072078, -0.091091\C, 0, -2.643594, -3.183384, 2.940061\H, 0, -3.191135, -1.039262, 2.995962\H, 0, -4.529846, -2.020608, 2.327085\H, 0, -2.290906, -3.146363, 3.981607\H, 0, -3.193107, -4.126875, 2.795086\H, 0, -0.72477, -2.345975, 2.178245\H, 0, -1.217391, -3.800095, 1.257149\\Version=ES64L-G09RevD.01\State=1-A\HF=-2317.4309742\RMSD=7.995e-09\Dipole=1.0148819, 0.111501, 3.231874\Quadrupole=-31.5959838, 26.9113305, 4.6846533, -2.9493088, -20.1761419, -6.1039802\PG=C01 [X(C21H25N1O11Rh2S1)]\@

B-1INT3

1\1\GINB-A757\SP\RBPW91\GenECP\C21H25N1O11Rh2S1\SIOC001\14-Mar-2018\O\
#p genecp scrf=(iefpcm, solvent=dichloromethane, smd) bpw91\\Title Card
Required\\0, 1\C, 0, -3.241255, -2.633971, 0.378857\H, 0, -3.793071, -3.290076, 1.069185\H, 0, -2.984191, -3.213848, -0.523591\O, 0, -4.169703, -1.575485, 0.027402\S, 0, -3.741192, -0.868622, -1.446011\C, 0, -1.508808, -0.899464, 0.245496\Rh, 0, 0.542084, -0.045714, -0.020737\C, 0, -1.838161, 0.406651, 0.04107\N, 0, -2.012562, -0.437989, -1.157396\C, 0, -2.300386, 1.708245, 0.443846\C, 0, -2.346472, 2.07699, 1.81037\C, 0, -2.70855, 2.636626, -0.544257\C, 0, -2.81074, 3.342973, 2.176548\H, 0, -2.022853, 1.363484, 2.570603\C, 0, -3.169628, 3.900475, -0.166744\H, 0, -2.673506, 2.344341, -1.59453\C, 0, -3.223699, 4.256727, 1.191273\H, 0, -2.856284, 3.619048, 3.233661\H, 0, -3.494604, 4.609261, -0.933053\H, 0, -3.591357, 5.244636, 1.482842\C, 0, -1.962291, -2.084345, 1.050475\C, 0, -2.127264, -1.855744, 2.591737\C, 0, -1.021678, -3.296384, 1.383257\O, 0, -4.602013, 0.317513, -1.559231\O, 0, -3.709592, -1.897687, -2.497206\O, 0, 2.853648, 2.029799, 0.634267\C, 0, 1.724984, 2.392013, 1.118625\O, 0, 0.612455, 1.752677, 1.012904\O, 0, 3.283411, -0.682102, 1.466869\C, 0, 2.268566, -1.051973, 2.150939\O, 0, 1.031987, -0.946077, 1.8023\O, 0, 3.034962, -1.558338, -1.310382\C, 0, 1.932898, -2.186718, -1.491497\O, 0, 0.771508, -1.825884, -1.072735\O, 0, 2.601633, 1.156688, -2.117707\C, 0, 1.382541, 1.323555, -2.477916\O, 0, 0.338596, 0.949765, -1.827314\C, 0, 1.690048, 3.680159, 1.915169\C, 0, 1.131698, 2.037863, -3.789859\C, 0, 2.532254, -1.686041, 3.50288\C, 0, 1.985902, -3.481632,

-2.276393\H,0,1.974012,-1.14825,4.284882\H,0,2.177587,-2.729072,3.501299\H,0,3.60565,-1.666471,3.731107\H,0,3.019353,-3.711647,-2.566129\H,0,1.575676,-4.304726,-1.670909\H,0,1.357509,-3.391328,-3.176342\H,0,2.510522,4.340353,1.602733\H,0,0.720864,4.182337,1.791917\H,0,1.821558,3.447753,2.985382\H,0,0.411597,1.467397,-4.395263\H,0,0.688111,3.026764,-3.590159\H,0,2.072677,2.168106,-4.340147\Rh,0,2.948952,0.232326,-0.332261\C,0,-1.576085,-3.288808,2.836687\H,0,-1.423723,-1.091079,2.949988\H,0,-3.143643,-1.611977,2.940241\H,0,-0.840878,-3.398974,3.647558\H,0,-2.374177,-4.031763,2.992946\H,0,0.032092,-3.003066,1.333692\H,0,-1.176907,-4.204984,0.778209\\Version=ES64L-G09RevD.01\State=1-A\HF=-2317.440065\RMSD=4.432e-09\Dipole=1.4000669,0.1485612,2.8011014\Quadrupole=-33.8183377,24.2006202,9.6177175,-5.9833276,-12.2692092,-4.680794\PG=C01 [X(C21H25N1O11Rh2S1)]\@e

B-¹Ts4

1\1\GINB-A763\SP\RBPW91\GenECP\C21H25N1O11Rh2S1\SI0C001\15-Mar-2018\0\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\\Title Card Required\\0,1\C,0,-2.7747,-2.758531,0.501959\H,0,-3.160457,-3.555228,1.156574\H,0,-2.282756,-3.222474,-0.36875\O,0,-3.945022,-2.016441,0.084765\S,0,-3.753764,-1.267358,-1.409346\C,0,-1.327843,-0.717149,0.421821\Rh,0,0.618208,-0.062734,-0.006363\C,0,-2.129326,0.320255,-0.057331\N,0,-2.26951,-0.452852,-1.201881\C,0,-2.608098,1.631958,0.283755\C,0,-2.30222,2.205222,1.544609\C,0,-3.411829,2.350326,-0.637295\C,0,-2.818726,3.45605,1.886127\H,0,-1.652967,1.662572,2.234235\C,0,-3.921099,3.602354,-0.286121\H,0,-3.639225,1.904163,-1.606468\C,0,-3.630325,4.154889,0.973649\H,0,-2.588693,3.893456,2.861429\H,0,-4.548642,4.150828,-0.993281\H,0,-4.033257,5.135023,1.244345\C,0,-1.771952,-1.876394,1.277435\C,0,-2.330684,-1.48828,2.698649\C,0,-0.750031,-2.822056,1.997256\O,0,-4.899532,-0.34616,-1.485413\O,0,-3.526362,-2.283871,-2.444529\O,0,2.672334,2.340142,-0.067539\C,0,1.479715,2.730639,0.183796\O,0,0.43804,1.978518,0.288673\O,0,3.344441,0.11205,1.635104\C,0,2.337611,-0.097166,2.395276\O,0,1.107231,-0.212205,2.026059\O,0,3.294201,-1.651889,-0.690383\C,0,2.267563,-2.417221,-0.640982\O,0,1.060773,-2.06398,-0.365306\O,0,2.612175,0.575924,-2.364149\C,0,1.401697,0.44047,-2.765507\O,0,0.379729,0.176333,-2.028236\C,0,1.257865,4.221055,0.340779\C,0,1.125198,0.62756,-4.242554\C,0,2.610779,-0.250741,3.879421\C,0,2.479425,-3.888485,-0.938914\H,0,1.860666,0.300464,4.465458\H,0,2.536803,-1.315053,4.158103\H,0,3.619708,0.108732,4.120447\H,0,3.542166,-4.093354,-1.121499\H,0,2.121406,-4.498527,-0.09505\H,0,1.889753,-4.173063,-1.824799\H,0,2.170468,4.702364,0.718382\H,0,1.024064,4.65413,-0.646323\H,0,0.409195,4.41982,1.008828\H,0,0.382292,-0.107512,-4.583671\H,0,0.702353,1.632228,-4.409\H,0,2.054607,0.534353,-4.819911\Rh,0,3.003028,0.344405,-0.370506\C,0,-1.625432,-2.744316,3.280417\H,0,-1.864483,-0.564218,3.070314\H,0,-3.425166,-1.399396,2.778341\H,0,-1.091417,-2.605687,4.232391\H,0,-2.30

8348,-3.601425,3.3899\H,0,0.219061,-2.329474,2.127052\H,0,-0.595538,-3.810217,1.534901\\Version=ES64L-G09RevD.01\State=1-A\HF=-2317.43524\RM SD=3.716e-09\Dipole=1.1005037,1.2482808,2.8974894\Quadrupole=-33.6095087,24.6340408,8.9754678,-16.6225769,-11.7379096,-5.8463552\PG=C01 [X(C21H25N1O11Rh2S1)]\@

B-¹INT4

1\1\GINB-A763\SP\RBPW91\GenECP\C21H25N1O11Rh2S1\SI0C001\15-Mar-2018\0\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\\Title Card
Required\0,1\C,0,-2.7747,-2.758531,0.501959\H,0,-3.160457,-3.555228,
1.156574\H,0,-2.282756,-3.222474,-0.36875\O,0,-3.945022,-2.016441,0.08
4765\S,0,-3.753764,-1.267358,-1.409346\C,0,-1.327843,-0.717149,0.42182
1\Rh,0,0.618208,-0.062734,-0.006363\C,0,-2.129326,0.320255,-0.057331\N
,0,-2.26951,-0.452852,-1.201881\C,0,-2.608098,1.631958,0.283755\C,0,-2
.30222,2.205222,1.544609\C,0,-3.411829,2.350326,-0.637295\C,0,-2.81872
6,3.45605,1.886127\H,0,-1.652967,1.662572,2.234235\C,0,-3.921099,3.602
354,-0.286121\H,0,-3.639225,1.904163,-1.606468\C,0,-3.630325,4.154889,
0.973649\H,0,-2.588693,3.893456,2.861429\H,0,-4.548642,4.150828,-0.993
281\H,0,-4.033257,5.135023,1.244345\C,0,-1.771952,-1.876394,1.277435\C
,0,-2.330684,-1.48828,2.698649\C,0,-0.750031,-2.822056,1.997256\O,0,-4
.899532,-0.34616,-1.485413\O,0,-3.526362,-2.283871,-2.444529\O,0,2.672
334,2.340142,-0.067539\C,0,1.479715,2.730639,0.183796\O,0,0.43804,1.97
8518,0.288673\O,0,3.344441,0.11205,1.635104\C,0,2.337611,-0.097166,2.3
95276\O,0,1.107231,-0.212205,2.026059\O,0,3.294201,-1.651889,-0.690383
\C,0,2.267563,-2.417221,-0.640982\O,0,1.060773,-2.06398,-0.365306\O,0,
2.612175,0.575924,-2.364149\C,0,1.401697,0.44047,-2.765507\O,0,0.37972
9,0.176333,-2.028236\C,0,1.257865,4.221055,0.340779\C,0,1.125198,0.627
56,-4.242554\C,0,2.610779,-0.250741,3.879421\C,0,2.479425,-3.888485,-0
.938914\H,0,1.860666,0.300464,4.465458\H,0,2.536803,-1.315053,4.158103
\H,0,3.619708,0.108732,4.120447\H,0,3.542166,-4.093354,-1.121499\H,0,2
.121406,-4.498527,-0.09505\H,0,1.889753,-4.173063,-1.824799\H,0,2.1704
68,4.702364,0.718382\H,0,1.024064,4.65413,-0.646323\H,0,0.409195,4.419
82,1.008828\H,0,0.382292,-0.107512,-4.583671\H,0,0.702353,1.632228,-4.
409\H,0,2.054607,0.534353,-4.819911\Rh,0,3.003028,0.344405,-0.370506\C
,0,-1.625432,-2.744316,3.280417\H,0,-1.864483,-0.564218,3.070314\H,0,-
3.425166,-1.399396,2.778341\H,0,-1.091417,-2.605687,4.232391\H,0,-2.30
8348,-3.601425,3.3899\H,0,0.219061,-2.329474,2.127052\H,0,-0.595538,-3
.810217,1.534901\\Version=ES64L-G09RevD.01\State=1-A\HF=-2317.43524\RM
SD=3.716e-09\Dipole=1.1005037,1.2482808,2.8974894\Quadrupole=-33.60950
87,24.6340408,8.9754678,-16.6225769,-11.7379096,-5.8463552\PG=C01 [X(C
21H25N1O11Rh2S1)]\@

B-¹TS5

1\1\GINB-A756\SP\RBPW91\GenECP\C21H25N1O11Rh2S1\SI0C001\14-Mar-2018\0\


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\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\Title Card
Required\0,1\C,0,-2.698093,-2.48758,1.630602\H,0,-3.228448,-2.688322
,2.577101\H,0,-2.088994,-3.38537,1.396125\O,0,-3.714398,-2.292015,0.65
7308\O,0,-4.267124,-2.466717,-1.780433\S,0,-3.114524,-2.130822,-0.9414
81\O,0,-1.857313,-2.898807,-1.03709\N,0,-2.952998,-0.461622,-1.038434\C
,0,-2.436898,0.229411,-0.034743\Rh,0,0.587578,0.088303,0.212258\Rh,0,
2.82424,0.062863,-0.789239\O,0,0.799259,-1.973753,0.378288\O,0,2.88510
6,-1.969137,-0.568606\O,0,1.546523,0.374762,2.039913\C,0,2.834247,0.44
5102,2.075217\O,0,3.627408,0.336264,1.079288\O,0,0.648878,2.145498,-0.
050147\O,0,2.718377,2.090466,-1.032145\O,0,-0.110115,-0.140077,-1.7190
42\C,0,0.712065,-0.251812,-2.701279\O,0,1.992045,-0.203535,-2.629444\C
,0,0.09329,-0.476868,-4.064695\C,0,3.456544,0.68038,3.439181\C,0,-1.45
0642,-0.265398,0.96871\C,0,1.861532,-2.550092,-0.065283\C,0,1.885115,-
4.063382,0.015962\C,0,1.672244,2.69306,-0.608808\C,0,1.633499,4.202395
,-0.750731\C,0,-2.85418,1.665176,-0.040458\C,0,-2.155462,2.69628,0.628
786\C,0,-4.065773,1.992877,-0.69844\C,0,-2.657393,4.003897,0.64564\H,0
,-1.185163,2.491833,1.080036\C,0,-4.558114,3.30137,-0.685572\H,0,-4.61
5733,1.197513,-1.204393\C,0,-3.860002,4.313301,-0.00751\H,0,-2.09711,4
.787277,1.164145\H,0,-5.498488,3.528819,-1.195328\H,0,-4.250743,5.3347
49,0.012305\H,0,1.065304,-4.471148,-0.596081\H,0,2.846525,-4.452163,-0
.343715\H,0,1.717123,-4.390597,1.054155\H,0,0.852391,-0.378929,-4.8517
45\H,0,-0.343741,-1.487827,-4.100398\H,0,-0.72461,0.240061,-4.229401\H
,0,1.853792,4.667579,0.224728\H,0,2.386442,4.536031,-1.47694\H,0,0.630
891,4.529999,-1.061218\H,0,4.550231,0.723955,3.357979\H,0,3.080098,1.6
24547,3.864077\H,0,3.170389,-0.129529,4.128995\C,0,-2.069509,0.169543,
2.742868\C,0,-1.667926,-1.392135,1.799172\C,0,-0.701666,-1.659589,2.97
3044\H,0,-3.101125,-0.127211,2.993972\H,0,-2.087784,1.22864,2.461842\H
,0,0.33308,-1.807867,2.644041\H,0,-1.02529,-2.541207,3.549576\C,0,-0.9
71969,-0.320533,3.695906\H,0,-0.095842,0.338006,3.665069\H,0,-1.326278
,-0.422842,4.733441\Version=ES64L-G09RevD.01\State=1-A\HF=-2317.42900
71\RMSD=7.841e-10\Dipole=-0.0790152,1.5467056,4.3887832\Quadrupole=-25
.0160001,11.7300446,13.2859554,-13.8375453,-8.8097622,-10.5017882\PG=C
01 [X(C21H25N1O11Rh2S1)]\@
```

B-1TS7

```
1\1\GINB-A761\SP\RBPW91\GenECP\C21H25N1O11Rh2S1\SIOC001\14-Mar-2018\0\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\Title Card
Required\0,1\O,0,-2.977938,-2.568476,0.749107\O,0,-4.806313,-2.56129
6,-0.981408\S,0,-3.372869,-2.267964,-0.948231\O,0,-2.414641,-3.035451,
-1.757286\N,0,-3.172017,-0.635342,-1.104746\C,0,-2.469112,0.124599,-0.
279497\Rh,0,0.589488,-0.054648,0.096892\Rh,0,2.951199,0.140897,-0.5132
32\O,0,0.478261,-1.628389,-1.216562\O,0,2.672707,-1.403454,-1.84039\O,
0,1.196311,-1.415133,1.557179\C,0,2.451793,-1.698046,1.663936\O,0,3.40
```

4137,-1.209532,0.96631\O,0,0.913635,1.531221,1.4132\O,0,3.128367,1.680
03,0.831905\O,0,0.199931,1.260982,-1.448442\C,0,1.179402,1.726331,-2.1
43175\O,0,2.423994,1.475749,-1.970398\C,0,0.80544,2.646143,-3.288424\C
,0,2.819147,-2.722421,2.722071\C,0,-1.446389,-0.2814,0.714452\C,0,-1.6
99422,-2.178191,1.03626\C,0,1.522983,-1.962607,-1.898717\C,0,1.35949,-
3.136773,-2.841575\C,0,2.093486,2.051604,1.482824\C,0,2.259604,3.24075
3,2.410679\C,0,-2.73398,1.586423,-0.401067\C,0,-2.004719,2.542175,0.34
2083\C,0,-3.794416,2.028313,-1.227745\C,0,-2.337445,3.9006,0.265363\H,
0,-1.1538,2.234167,0.952479\C,0,-4.112107,3.386529,-1.309037\H,0,-4.36
5412,1.288188,-1.791112\C,0,-3.387743,4.329271,-0.559828\H,0,-1.762032
,4.628608,0.8443\H,0,-4.934777,3.71125,-1.952148\H,0,-3.641787,5.39155
9,-0.619782\H,0,1.810762,-2.89702,-3.815913\H,0,1.896806,-4.009588,-2.
435066\H,0,0.29827,-3.388597,-2.961993\H,0,0.354934,2.050215,-4.099246
\H,0,0.052863,3.377146,-2.958474\H,0,1.695914,3.159831,-3.673902\H,0,2
.090293,4.169937,1.840843\H,0,1.531511,3.203078,3.232736\H,0,3.283779,
3.270352,2.8077\H,0,2.437922,-2.406168,3.705704\H,0,2.350708,-3.690396
,2.480813\H,0,3.908391,-2.848193,2.77072\C,0,-1.81985,-0.453806,2.0542
48\C,0,-3.155828,-0.252335,2.763345\C,0,-1.038943,-0.372645,3.364126\H
,0,-1.349485,-2.610833,1.979397\H,0,-0.959139,-2.352086,0.237077\C,0,-
2.33633,0.215124,4.00907\H,0,-0.136855,0.250942,3.322846\H,0,-0.770621
,-1.355865,3.782419\H,0,-2.299722,1.310597,4.093345\H,0,-2.637638,-0.2
13314,4.975599\H,0,-3.852313,0.456091,2.289665\H,0,-3.687452,-1.204151
,2.930143\\Version=ES64L-G09RevD.01\State=1-A\HF=-2317.4338322\RMSD=2.
373e-09\Dipole=0.0352157,1.7628316,3.2476896\Quadrupole=-28.7552047,12
.3225028,16.4327019,-20.6553495,-5.4990082,-9.1032239\PG=C01 [X(C21H25
N1O11Rh2S1)]\@

B-1PCI

1\1\GINB-A728\SP\RBPW91\GenECP\C21H25N1O11Rh2S1\SI0C001\20-Mar-2018\O\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\\Title Card
Required\\0,1\C,0,-2.575249,-2.572865,-2.017951\H,0,-3.254881,-3.2579
92,-2.561709\H,0,-1.576409,-3.046723,-1.995389\O,0,-2.567147,-1.39141,
-2.878775\O,0,-1.083482,0.960129,-3.313133\S,0,-1.506526,-0.01344,-2.0
93354\O,0,-0.246323,-0.977017,-1.269668\N,0,-3.158643,0.854186,-1.2625
33\C,0,-3.826562,0.089583,-0.431788\Rh,0,1.350166,-0.161146,-0.27029\R
h,0,3.293693,0.647053,0.927035\O,0,2.199767,-2.057028,-0.143434\O,0,4.
052485,-1.252793,1.001943\O,0,0.419252,-0.463171,1.563452\C,0,1.080125
, -0.168483,2.657879\O,0,2.294894,0.31645,2.694581\O,0,0.633232,1.75341
2,-0.312323\O,0,2.491368,2.538755,0.818162\O,0,2.372272,0.174687,-2.02
8878\C,0,3.584132,0.671221,-1.978682\O,0,4.230527,0.959426,-0.875125\C
,0,4.265966,0.955093,-3.290969\C,0,0.377587,-0.39406,3.973297\C,0,-3.5
73502,-1.288459,0.044052\C,0,3.358521,-2.215165,0.445047\C,0,3.947036,
-3.602048,0.456292\C,0,1.340808,2.720722,0.226814\C,0,0.76645,4.110392
,0.181169\C,0,-5.033863,0.814817,0.112734\C,0,-4.93848,2.172879,0.4942
91\C,0,-6.284216,0.155848,0.181994\C,0,-6.074358,2.854556,0.959835\H,0

, -3.972973, 2.675641, 0.424023\C, 0, -7.417334, 0.845737, 0.641233\H, 0, -6.363142, -0.88583, -0.136745\C, 0, -7.314853, 2.194363, 1.034273\H, 0, -5.991513, 3.900535, 1.262686\H, 0, -8.3806, 0.333124, 0.688781\H, 0, -8.197843, 2.72693, 1.394329\H, 0, 4.377203, -3.826713, -0.53414\H, 0, 4.740703, -3.670543, 1.210849\H, 0, 3.162344, -4.345578, 0.65573\H, 0, 5.353474, 1.003508, -3.151283\H, 0, 4.003873, 0.18281, -4.027183\H, 0, 3.916187, 1.924813, -3.683532\H, 0, 0.094157, 4.261888, 1.042807\H, 0, 1.573235, 4.852668, 0.238346\H, 0, 0.180668, 4.247217, -0.737784\H, 0, 1.07624, -0.242296, 4.805113\H, 0, -0.464471, 0.310245, 4.072799\H, 0, -0.035113, -1.413524, 4.009524\C, 0, -3.800669, -1.616466, 1.530134\C, 0, -3.04576, -2.373293, -0.609272\C, 0, -2.877548, -3.553271, 0.342553\C, 0, -3.727185, -3.165836, 1.581759\H, 0, -1.802404, -3.64633, 0.594772\H, 0, -3.183402, -4.51263, -0.110412\H, 0, -3.298453, -3.539236, 2.52413\H, 0, -4.741759, -3.589861, 1.484119\H, 0, -2.986452, -1.155334, 2.121534\H, 0, -4.748466, -1.219941, 1.923904\\Version=ES64L-G09RevD.01\\State=1-A\\HF=-2317.4584675\\RMSD=7.087e-09\\Dipole=-2.0901998, -1.4581842, 2.937364\\Quadrupole=13.6684037, 10.9427594, -24.6111631, 1.4961183, -22.7014641, 3.1122697\\PG=C01 [X(C21H25N1O11Rh2S1)]\\@

B-1P1

1\\1\\GINB-A765\\SP\\RBPW91\\6-311++G(d,p)\\C13H13N1O3S1\\SI0C001\\27-Mar-2018\\0\\#p 6-311++g(d,p) bpw91 scrf=(iefpcm, solvent=dichloromethane, smd)\\Title Card Required\\0, 1\C, 0, 2.535928, 0.807817, 1.105738\H, 0, 2.685104, 1.294814, 2.088525\H, 0, 3.490128, 0.903015, 0.549365\O, 0, 2.276346, -0.579825, 1.46599\O, 0, 2.451207, -3.12909, 0.18234\S, 0, 2.068059, -1.592818, -0.154795\O, 0, 2.855496, -0.795902, -1.35424\N, 0, 0.135483, -1.498077, -0.123209\C, 0, -0.374944, -0.28092, -0.085852\C, 0, 0.252785, 1.054941, -0.153421\C, 0, -1.876269, -0.350586, -0.001373\C, 0, -2.593004, -1.302379, -0.762443\C, 0, -2.572924, 0.493547, 0.896237\C, 0, -3.988752, -1.393088, -0.641354\H, 0, -2.047175, -1.957685, -1.442326\C, 0, -3.96719, 0.38973, 1.020316\H, 0, -2.017392, 1.209479, 1.506012\C, 0, -4.678486, -0.549441, 0.248938\H, 0, -4.536829, -2.123408, -1.240043\H, 0, -4.497585, 1.037812, 1.721259\H, 0, -5.763956, -0.623856, 0.34374\C, 0, -0.43225, 2.159008, -0.980473\C, 0, 1.459076, 1.499456, 0.327089\C, 0, 1.721194, 2.940051, -0.09792\C, 0, 0.340712, 3.447766, -0.592341\H, 0, 2.472897, 2.937707, -0.912744\H, 0, 2.142276, 3.553775, 0.717384\H, 0, 0.423896, 4.158856, -1.427907\H, 0, -0.182365, 3.961106, 0.232868\H, 0, -0.313143, 1.925595, -2.056354\H, 0, -1.512833, 2.23754, -0.792162\\Version=ES64L-G09RevD.01\\State=1-A\\HF=-1181.8472201\\RMSD=4.177e-09\\Dipole=-2.3197823, 3.7261835, 0.2567373\\Quadrupole=5.576447, -3.9614337, -1.6150133, 15.0400829, 2.9058281, 5.1891214\\PG=C01 [X(C13H13N1O3S1)]\\@

B-1PC3

1\\1\\GINB-A728\\SP\\RBPW91\\GenECP\\C21H25N1O11Rh2S1\\SI0C001\\20-Mar-2018\\0\\#p genecp scrf=(iefpcm, solvent=dichloromethane, smd) bpw91\\Title Card Required\\0, 1\\Rh, 0, -2.664824, 0.079294, -1.003609\O, 0, -2.201793, -1.677908, -1.959445\C, 0, -1.090492, -2.292338, -1.651062\O, 0, -0.212183, -1.86127, -0.772641\O, 0, -3.687277, -0.977673, 0.419523\C, 0, -3.022815, -1.428849, 1.4

47606\O,0,-1.738668,-1.240472,1.644449\O,0,-3.076977,1.836124,-0.03120
9\C,0,-2.272538,2.229774,0.921895\O,0,-1.205538,1.571442,1.312421\O,0,
-1.691205,1.137339,-2.448321\C,0,-0.413108,1.369861,-2.289836\O,0,0.28
1135,0.959573,-1.253159\N,0,3.318829,1.097591,-0.465058\C,0,-0.806814,
-3.607179,-2.330718\C,0,0.317532,2.134152,-3.355355\C,0,-3.779004,-2.2
14416,2.488077\C,0,-2.569491,3.533665,1.610233\S,0,2.904917,2.967818,-
0.02283\O,0,4.126091,3.539536,0.89689\O,0,2.434751,3.803798,-1.335297\
C,0,2.676906,0.159447,0.206251\O,0,1.357398,2.794683,1.047996\C,0,1.60
2831,1.671538,1.973997\H,0,0.746699,1.71891,2.656482\H,0,2.531871,1.86
7815,2.546143\C,0,1.689655,0.302002,1.297813\Rh,0,-0.602457,-0.116522,
0.28541\H,0,0.970246,1.450545,-3.923984\H,0,-0.400177,2.598538,-4.0429
79\H,0,0.964432,2.892367,-2.887885\H,0,0.255707,-3.864305,-2.23972\H,0
, -1.405718,-4.403599,-1.857465\H,0,-1.101145,-3.554335,-3.388495\H,0,-
4.811069,-2.380266,2.155916\H,0,-3.284103,-3.181234,2.667091\H,0,-3.78
731,-1.66354,3.442482\H,0,-1.816965,4.280435,1.308109\H,0,-3.569253,3.
890095,1.333818\H,0,-2.49707,3.414403,2.701547\C,0,3.237625,-1.16844,-
0.252013\C,0,2.917449,-1.681405,-1.525992\C,0,4.206767,-1.822917,0.543
67\C,0,3.525605,-2.865156,-1.97888\H,0,2.197774,-1.148728,-2.145783\C,
0,4.811924,-3.004363,0.085462\H,0,4.496697,-1.395415,1.506379\C,0,4.46
8303,-3.530697,-1.174677\H,0,3.277278,-3.256444,-2.967932\H,0,5.562499
, -3.502799,0.702724\H,0,4.947304,-4.444371,-1.533478\C,0,1.124192,-0.7
72512,1.994908\C,0,0.520445,-0.761262,3.411267\C,0,1.25721,-2.303704,2
.000598\C,0,0.654343,-2.322931,3.447191\H,0,1.137345,-0.221154,4.15065
5\H,0,-0.512471,-0.390863,3.470504\H,0,1.343509,-2.69893,4.217694\H,0,
-0.305684,-2.848214,3.529662\H,0,2.290762,-2.670615,1.918558\H,0,0.660
995,-2.808249,1.227325\\Version=ES64L-G09RevD.01\State=1-A\HF=-2317.43
1296\RMSD=8.542e-09\Dipole=-1.353928,-4.6152789,1.9892061\Quadrupole=-
14.9522343,-2.9812318,17.9334661,-27.4459262,-5.1335717,4.6267203\PG=C
01 [X(C21H25N1O11Rh2S1)]\@

B-1P3

1\1\GINB-A765\SP\RBPW91\6-311++G(d,p)\C13H13N1O3S1\SI0C001\27-Mar-2018
\0\#\p 6-311++g(d,p) bpw91 scrf=(iefpcm,solvent=dichloromethane,smd)\
Title Card Required\0,1\N,0,0.85171,-1.458635,-0.025168\S,0,2.749627,
-1.001881,-0.155053\O,0,3.515693,-1.773563,1.05547\O,0,3.23898,-1.1739
61,-1.693762\C,0,0.008613,-0.455826,0.167797\O,0,2.794831,0.87259,0.17
6927\C,0,1.696708,1.162574,1.142989\H,0,1.860083,2.211202,1.42713\H,0,
1.817152,0.53195,2.041878\C,0,0.354944,0.946957,0.476144\C,0,-1.415988
, -0.910659,0.122993\C,0,-1.819046,-1.877405,-0.829667\C,0,-2.350609,-0
.442417,1.077949\C,0,-3.1411,-2.347833,-0.839637\H,0,-1.089104,-2.2430
9,-1.553094\C,0,-3.668797,-0.924466,1.068307\H,0,-2.033329,0.279699,1.
832663\C,0,-4.068086,-1.873847,0.107939\H,0,-3.447435,-3.085107,-1.584
393\H,0,-4.381977,-0.566432,1.813906\H,0,-5.09542,-2.244493,0.101018\C
,0,-0.402206,2.004231,0.072674\C,0,-0.146477,3.513143,0.14173\C,0,-1.6
53836,2.191549,-0.788845\C,0,-1.266255,3.706403,-0.94489\H,0,-0.407487

,3.956927,1.1188\H,0,0.868199,3.846716,-0.127148\H,0,-2.054163,4.43114
2,-0.69832\H,0,-0.857085,3.943455,-1.937239\H,0,-2.594142,2.038461,-0.
234033\H,0,-1.704522,1.585147,-1.706114\\Version=ES64L-G09RevD.01\Stat
e=1-A\HF=-1181.8201313\RMSD=4.918e-09\Dipole=-4.578454,2.7172086,0.840
0116\Quadrupole=-8.7707277,6.9707009,1.8000268,11.0315225,2.6469502,4.
8431229\PG=C01 [X(C13H13N1O3S1)]\@

B-¹TS8

B-¹INT5

1\1\GINB-OM103\SP\RBPW91\GenECP\C21H25N1O11Rh2S1\WEIY\28-Apr-2018\0\#\#
p genecp bpw91 geom=check scrf=(iefpcm,solvent=dichloromethane,smd)\#T
itle Card Required\0,1\Rh,0,-0.6494438821,0.1674750421,0.0137260452\R
h,0,-2.8142115093,-0.9726887862,-0.1168518447\O,0,-1.5474127781,1.7295
601205,-1.0210758453\C,0,-2.7859665383,1.628813721,-1.3661315273\O,0,-
3.571334295,0.6514963433,-1.1123667082\O,0,-1.3068001661,0.9664108118,
1.8113156625\C,0,-2.4804001841,0.6531184695,2.251307091\O,0,-3.3196469
055,-0.1192150223,1.6760212479\O,0,0.0491510829,-1.516535506,0.9927675
618\C,0,-0.7396461259,-2.5228478457,1.164769244\O,0,-1.9776251941,-2.5
767999397,0.8449517602\O,0,-0.2604052511,-0.733846671,-1.8065436215\C,
0,-1.1182333557,-1.5235272293,-2.3496898736\O,0,-2.2809892247,-1.81316
98861,-1.891952772\C,0,-3.3466839558,2.7784171214,-2.1798625788\C,0,-0
.6864710503,-2.175907899,-3.6451594999\C,0,-2.872067002,1.2493190753,3
.5881210593\C,0,-0.1190406044,-3.7461059516,1.8056482284\C,0,3.2185383
838,1.6213440708,2.2799442857\C,0,2.3036504028,-0.2629993516,2.8424295
373\C,0,3.0563863783,0.2380409189,1.5531658108\C,0,2.3060839863,0.1478
446059,0.21712266\N,0,2.5752857138,-0.6764904687,-0.7615524673\S,0,3.7
982592365,-1.8430377992,-0.6362124239\O,0,4.2829599338,-1.8016999972,0
.9688688945\C,0,4.4308299955,-0.428162442,1.410276488\O,0,3.1896339273
, -3.1669597138,-0.8016312379\O,0,4.9112464765,-1.3996710525,-1.4920216
992\C,0,1.1397863708,1.034094013,-0.0050989382\C,0,1.3926743046,2.4193
134227,-0.3492292029\C,0,2.5624553504,2.7860367255,-1.0814981862\C,0,2
.796484064,4.1168761301,-1.4306344251\C,0,1.9008377859,5.1217428063,-1
.0226413138\C,0,0.7569394032,4.7847675763,-0.2781690063\C,0,0.48885414
55,3.4512362273,0.0375471792\H,0,2.425792247,2.330185011,2.0081047609\
H,0,4.1930573431,2.1217846264,2.1503448891\H,0,2.5360662033,-1.2929273
93,3.1526484664\H,0,1.2170988538,-0.1589873284,2.7277660586\H,0,4.9486
20225,-0.4910698005,2.3787535136\H,0,5.0778684946,0.1265104579,0.70617
70186\H,0,3.2549679923,2.0052820108,-1.4053045658\H,0,3.6838116921,4.3
771031929,-2.0142658011\H,0,2.096409362,6.1659986458,-1.2823864705\H,0
,0.0682964615,5.5686701994,0.0495089456\H,0,-0.3919537356,3.1820085455
,0.6202862189\H,0,-0.8530006475,-4.559935996,1.8652694578\H,0,0.75383

23173,-4.0637563517,1.214535417\H,0,0.239857135,-3.4974392261,2.816987
2664\H,0,-1.5334619828,-2.6951451927,-4.1122594932\H,0,-0.2762329714,-
1.4190133593,-4.3301411069\H,0,0.1180982882,-2.8984746553,-3.433619955
2\H,0,-2.3147109376,0.7410706407,4.3922405147\H,0,-2.6072687767,2.3164
842364,3.6234752014\H,0,-3.9480220864,1.1185658163,3.7622486338\H,0,-2
.932120785,3.7355970683,-1.8334178183\H,0,-3.0532602317,2.6478645873,-
3.2348504819\H,0,-4.443143069,2.7887063818,-2.1198720163\C,0,2.9211806
962,0.9207655836,3.6343557566\H,0,3.8360498371,0.6420229643,4.18053424
76\H,0,2.2545617857,1.453879038,4.3286992185\\Version=ES64L-G16RevA.03
\State=1-A\HF=-2317.468571\RMSD=9.008e-09\Dipole=-0.3904899,4.0539417,
2.0948836\Quadrupole=-18.2707177,8.103243,10.1674748,11.3416035,11.828
4013,-6.1216066\PG=C01 [X(C21H25N1O11Rh2S1)]\@

M-INT1

1\1\GINB-A754\SP\RBPW91\GenECP\C20H25N1O11Rh2S1\SI0C001\15-Mar-2018\0\
\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\\Title Card
Required\\0,1\Rh,0,-2.014466,-1.801624,0.311738\Rh,0,-1.538993,0.5366
71,-0.079517\O,0,-3.40731,-1.258705,1.701529\C,0,-3.600305,-0.008925,1
.92\O,0,-2.966801,0.958303,1.356348\O,0,-3.449249,-1.764203,-1.134456\
C,0,-3.659932,-0.647941,-1.733587\O,0,-3.044049,0.457272,-1.510348\O,0
, -0.617278,-2.308544,-1.083733\C,0,0.013287,-1.357216,-1.671715\O,0,-0
.165419,-0.099165,-1.469687\O,0,-0.568117,-1.813394,1.75334\C,0,0.0683
55,-0.72915,1.994978\O,0,-0.123569,0.401663,1.406071\N,0,-1.318168,2.3
70124,-0.554273\C,0,-4.676228,0.377866,2.909428\C,0,1.141536,-0.756207
,3.058579\C,0,-4.719049,-0.616177,-2.813242\C,0,1.079054,-1.732973,-2.
673408\S,0,0.06826,3.184222,-0.941837\O,0,0.144277,3.169522,-2.419562\
O,0,0.01171,4.46512,-0.194358\O,0,1.465076,2.379518,-0.472809\C,0,2.10
1697,2.78149,0.767605\H,0,1.883593,3.842385,0.966038\H,0,1.700331,2.16
2554,1.584137\C,0,3.637063,2.594661,0.639633\C,0,4.183809,3.446641,-0.
535002\C,0,4.259752,3.077157,1.979948\C,0,3.984201,1.178023,0.429735\C
,0,4.339899,0.016875,0.258369\C,0,4.754682,-1.328426,0.010496\C,0,5.10
1915,-1.740223,-1.30195\C,0,4.833276,-2.27708,1.060755\C,0,5.50413,-3.
057703,-1.549969\H,0,5.056085,-1.011237,-2.114779\C,0,5.234679,-3.5926
03,0.802525\H,0,4.58017,-1.967318,2.077692\C,0,5.569868,-3.989612,-0.5
01764\H,0,5.769827,-3.358188,-2.567592\H,0,5.288048,-4.311923,1.624753
\H,0,5.883085,-5.018404,-0.699523\H,0,0.83422,-2.697385,-3.139383\H,0,
1.182828,-0.946572,-3.433051\H,0,2.042537,-1.834807,-2.147422\H,0,1.20
7262,-1.755816,3.506758\H,0,2.107508,-0.482691,2.605628\H,0,0.912944,-
0.011961,3.837538\H,0,-4.962503,-0.48816,3.520453\H,0,-4.325768,1.2017
95,3.547703\H,0,-5.560465,0.73725,2.357789\H,0,-5.399796,0.231397,-2.6
4382\H,0,-4.236108,-0.460121,-3.791218\H,0,-5.280038,-1.559532,-2.8273
\H,0,5.353133,2.953272,1.956292\H,0,4.034049,4.144123,2.143462\H,0,3.8
69469,2.501411,2.834563\H,0,5.277539,3.34274,-0.607873\H,0,3.735402,3.
131171,-1.487491\H,0,3.943027,4.510484,-0.371145\\Version=ES64L-G09Rev

D.01\State=1-A\HF=-2279.326949\RMSD=6.510e-09\Dipole=-0.0599677,-3.240
258,1.9242852\Quadrupole=15.5787755,-24.3606713,8.7818958,1.4034667,0.
9387323,15.0374202\PG=C01 [X(C20H25N1O11Rh2S1)]\@

M-1TS1

1\1\GINB-A754\SP\RBPW91\GenECP\C20H25N1O11Rh2S1\SIOC001\15-Mar-2018\0\
\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\Title Card
Required\0,1\0,0,3.251192,0.705515,-1.627332\C,0,2.371298,0.160814,-
2.386628\0,0,1.225816,-0.296109,-2.019863\0,0,1.933515,2.665145,0.0344
27\C,0,0.689981,2.676568,-0.277621\0,0,-0.064648,1.636296,-0.358975\0,
0,2.338861,0.989974,2.360896\C,0,1.210242,0.513684,2.744153\0,0,0.3284
71,-0.057884,2.00186\0,0,3.747071,-0.908275,0.704971\C,0,3.015469,-1.9
60788,0.618791\0,0,1.762813,-1.984386,0.342036\C,0,2.702308,0.013012,-
3.855532\C,0,3.672879,-3.299033,0.874582\C,0,0.050688,4.00549,-0.60336
4\C,0,0.861872,0.66056,4.211451\H,0,-0.965399,4.05357,-0.188038\H,0,0.
669159,4.826936,-0.217939\H,0,-0.031598,4.103948,-1.698426\H,0,1.77342
4,0.796214,4.808704\H,0,0.221086,1.548487,4.342108\H,0,0.29871,-0.2162
07,4.560582\H,0,2.956784,-1.039654,-4.061123\H,0,1.823543,0.264936,-4.
466425\H,0,3.555992,0.649627,-4.12251\H,0,4.75822,-3.176013,0.98376\H,
0,3.258359,-3.741447,1.794603\H,0,3.448011,-3.987613,0.046301\Rh,0,2.8
32672,0.871629,0.374121\C,0,-2.761325,-3.349627,0.095558\H,0,-3.274592
, -4.321401,0.006883\H,0,-1.733063,-3.522776,0.443584\0,0,-2.761888,-2.
778006,-1.227349\S,0,-1.353825,-1.961829,-1.673101\N,0,-0.874562,-1.31
8974,-0.208073\Rh,0,0.712798,-0.224664,-0.032158\C,0,-3.542892,-2.4408
93,1.099449\C,0,-5.067723,-2.70798,0.946613\C,0,-3.073489,-2.77532,2.5
36483\0,0,-1.834382,-1.041718,-2.722044\0,0,-0.338861,-2.996516,-2.001
35\C,0,-3.318835,-1.019747,0.780323\C,0,-3.444203,0.177926,0.51249\C,0
, -3.641614,1.541015,0.163199\C,0,-3.732881,2.544225,1.162796\C,0,-3.80
4459,1.907973,-1.199103\C,0,-3.990186,3.872395,0.807212\H,0,-3.609894,
2.262446,2.211386\C,0,-4.056009,3.239737,-1.541283\H,0,-3.714819,1.137
144,-1.967221\C,0,-4.154515,4.225211,-0.543595\H,0,-4.06902,4.63606,1.
586394\H,0,-4.179786,3.511369,-2.593438\H,0,-4.361398,5.263859,-0.8169
11\H,0,-5.385613,-2.542521,-0.094068\H,0,-5.652303,-2.042232,1.600308\
H,0,-2.011243,-2.518094,2.665578\H,0,-3.663544,-2.216379,3.279776\H,0,
-5.292206,-3.752501,1.223266\H,0,-3.205149,-3.852743,2.736611\Version
=ES64L-G09RevD.01\State=1-A\HF=-2279.3193386\RMSD=2.807e-09\Dipole=0.2
878269,1.5682255,2.4717609\Quadrupole=-6.8746406,9.7296695,-2.8550289,
-10.7025528,-11.8895361,-14.0745851\PG=C01 [X(C20H25N1O11Rh2S1)]\@

M-1INT2

1\1\GINB-A764\SP\RBPW91\GenECP\C20H25N1O11Rh2S1\SIOC001\15-Mar-2018\0\
\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\Title Card
Required\0,1\0,0,-2.296519,2.599749,-0.346197\C,0,-1.053017,2.84345,
-0.154165\0,0,-0.12309,1.974096,0.038383\0,0,-2.56362,0.529094,-2.3449

99\C,0,-1.396158,0.184747,-2.744418\O,0,-0.387075,-0.10985,-1.999939\O
,0,-3.450243,-1.339701,-0.284353\C,0,-2.534651,-2.220154,-0.112174\O,0
,-1.274336,-1.99637,0.027641\O,0,-3.185723,0.741437,1.703017\C,0,-2.18
5305,0.471139,2.460363\O,0,-1.007896,0.125554,2.074705\C,0,-0.640648,4
.302796,-0.122041\C,0,-2.39366,0.579638,3.957726\C,0,-1.18126,0.091611
,-4.243788\C,0,-2.975235,-3.669203,-0.034421\H,0,-1.989539,0.607295,-4
.778815\H,0,-0.207903,0.525244,-4.517061\H,0,-1.174825,-0.968076,-4.54
8874\H,0,-3.982513,-3.788995,-0.454848\H,0,-2.261165,-4.316927,-0.5638
06\H,0,-2.990827,-3.984514,1.022132\H,0,-1.226208,4.877018,-0.854127\H
,0,-0.854852,4.716954,0.877567\H,0,0.433876,4.407823,-0.322449\H,0,-1.
985307,-0.311241,4.457683\H,0,-1.844633,1.454892,4.342141\H,0,-3.46054
4,0.692799,4.190691\Rh,0,-2.917024,0.642541,-0.327195\C,0,2.443186,-3.
337228,0.066349\H,0,2.950987,-4.310488,-0.020195\H,0,1.376052,-3.51123
6,0.28267\O,0,3.077415,-2.654918,1.180661\S,0,2.038353,-1.532807,1.948
112\N,0,1.468722,-0.603065,0.314051\Rh,0,-0.626511,-0.030102,0.061463\
C,0,2.619083,0.09139,-0.330376\C,0,2.332822,-1.115327,-0.769106\C,0,3.
335,1.331103,-0.233226\C,0,4.361342,1.616109,-1.167466\C,0,3.038888,2.
260134,0.790939\C,0,5.070704,2.816334,-1.079074\H,0,4.588109,0.896526,
-1.958184\C,0,3.765853,3.451829,0.875298\H,0,2.245169,2.035217,1.50351
2\C,0,4.77723,3.735381,-0.056948\H,0,5.857637,3.035687,-1.805622\H,0,3
.540837,4.16458,1.673053\H,0,5.338258,4.671377,0.012491\C,0,2.609474,-
2.499857,-1.242076\C,0,4.058745,-2.579188,-1.769067\C,0,1.591744,-2.99
0224,-2.297854\H,0,4.778446,-2.298175,-0.984897\H,0,4.20085,-1.912434,
-2.634755\H,0,1.71725,-2.437802,-3.241179\H,0,0.560321,-2.846107,-1.94
5918\O,0,2.945336,-0.701042,2.759741\O,0,0.897114,-2.25925,2.52742\H,0
,4.281323,-3.608189,-2.096197\H,0,1.757858,-4.061884,-2.50073\\Version
=ES64L-G09RevD.01\State=1-A\HF=-2279.3678027\RMSD=3.785e-09\Dipole=2.1
716619,-0.1981423,-2.7068479\Quadrupole=-10.4318892,16.100665,-5.66877
58,8.8923331,-20.3535765,13.5447471\PG=C01 [X(C20H25N1O11Rh2S1)]\@

M-INT3

1\1\GINB-A755\SP\RBPW91\GenECP\C20H25N1O11Rh2S1\SI0C001\15-Mar-2018\O\
\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\\Title Card
Required\\0,1\C,0,-4.399113,-2.750073,0.714627\H,0,-4.863975,-3.48045
7,1.395318\H,0,-4.052777,-3.281409,-0.1882\O,0,-5.443781,-1.807952,0.3
69477\S,0,-5.141528,-0.994016,-1.109361\C,0,-3.046523,-0.795009,0.5829
07\Rh,0,1.219168,-0.166536,0.082011\N,0,-3.344577,-0.567311,-0.866363\
C,0,-3.162488,0.46228,0.235748\C,0,-3.172076,1.891616,0.333235\C,0,-2.
861208,2.532549,1.558352\C,0,-3.497244,2.67163,-0.801625\C,0,-2.874046
,3.927165,1.637225\H,0,-2.608518,1.93023,2.434403\C,0,-3.513243,4.0666
07,-0.706971\H,0,-3.746957,2.169934,-1.738372\C,0,-3.201249,4.698062,0
.507897\H,0,-2.633332,4.41735,2.584577\H,0,-3.772486,4.66425,-1.584962
\H,0,-3.21558,5.789267,0.577096\C,0,-3.206838,-2.01982,1.414272\C,0,-3
.572519,-1.622706,2.86046\C,0,-1.953555,-2.927026,1.374776\H,0,-4.5089

02,-1.044375,2.881466\H,0,-2.773033,-1.017255,3.317002\H,0,-1.104895,-
2.448316,1.886362\H,0,-1.649327,-3.144718,0.339437\O,0,-6.047734,0.168
153,-1.059556\O,0,-5.179954,-1.966537,-2.215809\O,0,3.511738,1.838341,
0.696719\C,0,2.393143,2.227219,1.197237\O,0,1.269705,1.607293,1.109753
\O,0,3.920712,-0.934249,1.411029\C,0,2.920434,-1.341768,2.107324\O,0,1
.677993,-1.164656,1.822708\O,0,3.505216,-1.706731,-1.362322\C,0,2.3793
71,-2.320085,-1.465037\O,0,1.261753,-1.936686,-0.957173\O,0,3.096108,1
.060694,-2.07574\C,0,1.85459,1.237125,-2.363444\O,0,0.853463,0.834186,
-1.664409\C,0,2.403478,3.544907,1.942917\C,0,1.540792,2.012384,-3.6245
92\C,0,3.234614,-2.128106,3.362698\C,0,2.362726,-3.592996,-2.283701\H,
0,3.318974,-3.197749,3.106952\H,0,4.194214,-1.802628,3.787362\H,0,2.42
8712,-2.013451,4.10059\H,0,3.346909,-4.080293,-2.254855\H,0,1.583099,-
4.274996,-1.917419\H,0,2.132298,-3.342785,-3.332872\H,0,3.235249,3.561
199,2.663176\H,0,2.569378,4.367163,1.227992\H,0,1.449206,3.704103,2.46
1153\H,0,1.406947,3.077147,-3.369969\H,0,2.3682,1.929407,-4.342277\H,0
,0.604301,1.649524,-4.07051\Rh,0,3.551197,0.068204,-0.340085\H,0,-2.16
8449,-3.881589,1.884441\H,0,-3.705212,-2.527772,3.476486\\Version=ES64
L-G09RevD.01\State=1-A\HF=-2279.3583636\RMSD=7.924e-09\Dipole=2.057882
3,0.2477122,2.5332237\Quadrupole=-45.6577503,31.3220633,14.335687,-5.1
028753,-15.4409781,-7.6364758\PG=C01 [X(C20H25N1O11Rh2S1)]\@

M-INT4

1\1\GINB-A761\SP\RBPW91\GenECP\C20H25N1O11Rh2S1\SI0C001\15-Mar-2018\0\
\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\\Title Card
Required\\0,1\C,0,-3.270354,-2.601246,1.117432\H,0,-3.799423,-3.01038
3,1.992127\H,0,-3.128733,-3.41003,0.382398\O,0,-4.163125,-1.603003,0.5
62728\S,0,-3.774698,-1.286393,-1.052956\C,0,-1.504231,-0.971811,0.5256
34\Rh,0,0.521066,-0.106138,0.046434\C,0,-1.860249,0.272079,0.102347\N,
0,-2.045535,-0.789397,-0.916074\C,0,-2.344178,1.618429,0.261277\C,0,-2
.355123,2.247789,1.53028\C,0,-2.81021,2.327045,-0.872701\C,0,-2.841754
,3.551457,1.65886\H,0,-1.982201,1.706859,2.401277\C,0,-3.29389,3.63065
7,-0.732156\H,0,-2.802128,1.8351,-1.845765\C,0,-3.312927,4.245436,0.53
0851\H,0,-2.859655,4.028604,2.642687\H,0,-3.663954,4.167774,-1.609522\
H,0,-3.698352,5.263361,0.63773\C,0,-1.893284,-2.012253,1.561081\C,0,-2
.027702,-1.318417,2.935216\C,0,-0.919808,-3.20959,1.636639\O,0,-4.6437
73,-0.165256,-1.436827\O,0,-3.761666,-2.544323,-1.816924\O,0,2.781363,
2.077149,0.491006\C,0,1.656913,2.435402,0.987734\O,0,0.563276,1.756105
,0.961464\O,0,3.355949,-0.578108,1.431233\C,0,2.386862,-0.920471,2.191
388\O,0,1.133003,-0.865792,1.899519\O,0,3.00031,-1.60074,-1.275665\C,0
,1.918643,-2.28458,-1.351453\O,0,0.764962,-1.940648,-0.899307\O,0,2.44
981,1.05782,-2.198399\C,0,1.213441,1.139165,-2.525994\O,0,0.212251,0.7
6002,-1.814283\C,0,1.603452,3.772294,1.698493\C,0,0.883194,1.736059,-3
.878373\C,0,2.735127,-1.424843,3.57827\C,0,1.997987,-3.643849,-2.01653
2\H,0,2.437902,-0.672605,4.32735\H,0,2.183106,-2.350188,3.80147\H,0,3.

815459,-1.602374,3.65836\H,0,2.922614,-3.728498,-2.602605\H,0,1.994112
, -4.429964, -1.243333\H,0,1.119857, -3.802055, -2.659204\H,0,2.390509, 4.4
36126, 1.315761\H,0,0.614079, 4.233132, 1.573422\H,0,1.775537, 3.61737, 2.7
76931\H,0,0.294568, 1.015305, -4.466883\H,0,0.264291, 2.637275, -3.745423\
H,0,1.803698, 1.995759, -4.41698\Rh,0,2.900244, 0.235184, -0.3875\H,0, -1.0
86296, -0.821574, 3.212149\H,0, -2.839337, -0.574183, 2.920258\H,0, -2.26272
4, -2.068619, 3.709644\H,0, 0.047659, -2.891587, 2.042865\H,0, -1.343368, -3.
986817, 2.2963\H,0, -0.752612, -3.645099, 0.64068\\Version=ES64L-G09RevD.0
1\State=1-A\HF=-2279.3561063\RMSD=4.368e-09\Dipole=1.4138922,0.677945,
2.6735569\Quadrupole=-33.5458209,20.1262684,13.4195525,-10.4980042,-9.
2439197,-7.0429545\PG=C01 [X(C20H25N1O11Rh2S1)]\@

M-1TS2

1\1\GINB-A764\SP\RBPW91\GenECP\C20H25N1O11Rh2S1\SIOC001\15-Mar-2018\0\
\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\\Title Card
Required\\0,1\C,0,-2.834207,-2.678313,1.179976\H,0,-3.211639,-3.31363
, 1.997622\H,0,-2.442065,-3.326958,0.379948\O,0,-3.979615,-1.944839,0.7
08418\S,0,-3.870908,-1.539658,-0.929518\C,0,-1.275881,-0.735556,0.7150
03\Rh,0,0.609473,-0.137744,0.083551\C,0,-2.138995,0.144702,0.037386\N,
0,-2.37483,-0.766237,-0.972128\C,0,-2.610867,1.504115,0.158205\C,0,-2.
376441,2.261907,1.333329\C,0,-3.366547,2.068824,-0.900006\C,0,-2.91431
, 3.544645,1.455024\H,0,-1.77833,1.83221,2.138194\C,0,-3.892248,3.35620
9,-0.772772\H,0,-3.536974,1.478728,-1.801522\C,0,-3.671648,4.093183,0.
403965\H,0,-2.744403,4.123112,2.367116\H,0,-4.47911,3.787109,-1.587968
\H,0,-4.089868,5.099063,0.502847\C,0,-1.690832,-1.777724,1.746767\C,0,
-2.207667,-1.012923,2.997584\C,0,-0.571662,-2.757507,2.158168\O,0,-5.0
03165,-0.61716,-1.119452\O,0,-3.752428,-2.761489,-1.736989\O,0,2.58339
1,2.332688,-0.12966\C,0,1.419892,2.675073,0.278279\O,0,0.413191,1.8903
32,0.46206\O,0,3.484868,0.111143,1.47032\C,0,2.561672,-0.153554,2.3147
53\O,0,1.309776,-0.314952,2.055751\O,0,3.259619,-1.633136,-0.85177\C,0
, 2.258775,-2.426273,-0.749292\O,0,1.063625,-2.110061,-0.388788\O,0,2.3
73718,0.589525,-2.435519\C,0,1.135532,0.442205,-2.730269\O,0,0.188456,
0.14838,-1.909057\C,0,1.204808,4.13828,0.608748\C,0,0.724849,0.648729,
-4.172835\C,0,2.967513,-0.299845,3.768837\C,0,2.490909,-3.889404,-1.07
0061\H,0,2.377212,0.387726,4.3944\H,0,2.755192,-1.324411,4.114001\H,0,
4.037515,-0.087615,3.890231\H,0,3.490505,-4.032638,-1.500382\H,0,2.402
161,-4.488945,-0.149493\H,0,1.721605,-4.244882,-1.772125\H,0,1.408074,
4.300416,1.680757\H,0,1.900066,4.761519,0.03007\H,0,0.165287,4.431693,
0.409504\H,0,-0.014885,-0.109571,-4.467087\H,0,0.250223,1.638359,-4.27
7781\H,0,1.60406,0.604963,-4.829155\Rh,0,2.942322,0.350978,-0.48704\H,
0,-1.423901,-0.354617,3.403271\H,0,-3.101511,-0.41508,2.76477\H,0,-2.4
73265,-1.743074,3.781477\H,0,0.255544,-2.219637,2.636896\H,0,-0.977081
, -3.492147, 2.875393\H,0, -0.174196, -3.293143, 1.285956\\Version=ES64L-G0
9RevD.01\State=1-A\HF=-2279.3492286\RMSD=7.354e-09\Dipole=1.5120961,1.

7705922,2.6938178\Quadrupole=-35.0858249,20.9536996,14.1321253,-20.739
273,-7.0057339,-6.525536\PG=C01 [X(C20H25N1O11Rh2S1)]\@

M-¹TS3

1\1\GINB-A743\SP\RBPW91\GenECP\C20H25N1O11Rh2S1\SIOC001\15-Mar-2018\0\
\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\Title Card
Required\0,1\C,0,3.888872,2.301285,0.878653\H,0,4.555474,2.679367,1.
667771\H,0,3.674018,3.123056,0.174979\O,0,4.644498,1.264643,0.202843\S
,0,3.954348,0.897701,-1.297773\C,0,2.039525,0.771069,0.486251\Rh,0,-0.
577337,0.036937,0.016638\C,0,1.490197,-0.463638,0.213545\N,0,2.248345,
0.772632,-0.882933\C,0,1.94657,-1.852139,0.300998\C,0,2.567888,-2.3598
01,1.464866\C,0,1.740106,-2.713534,-0.801183\C,0,2.972073,-3.698934,1.
521265\H,0,2.719522,-1.709612,2.327519\C,0,2.177458,-4.040397,-0.74928
3\H,0,1.252698,-2.314274,-1.691652\C,0,2.787623,-4.539808,0.413022\H,0
,3.448089,-4.081582,2.428495\H,0,2.037512,-4.690422,-1.617557\H,0,3.12
1634,-5.580466,0.453816\C,0,2.58042,1.733785,1.510764\C,0,2.874456,1.0
21103,2.846475\C,0,1.60465,2.91944,1.729144\O,0,4.514177,-0.40627,-1.6
66095\O,0,4.070001,2.066667,-2.183619\O,0,-3.205617,-1.747709,0.430815
\C,0,-2.131428,-2.362294,0.765505\O,0,-0.934085,-1.896911,0.704672\O,0
, -3.105563,0.817369,1.733081\C,0,-2.023184,0.922932,2.406157\O,0,-0.82
8501,0.685023,1.980526\O,0,-2.786665,2.102996,-0.879263\C,0,-1.604446,
2.582657,-0.995319\O,0,-0.505536,1.980832,-0.696709\O,0,-2.831489,-0.4
64946,-2.149933\C,0,-1.657411,-0.719979,-2.596323\O,0,-0.550245,-0.608
145,-1.948566\C,0,-2.275904,-3.768839,1.311685\C,0,-1.552585,-1.228015
, -4.020311\C,0,-2.143109,1.388991,3.844665\C,0,-1.472875,3.998149,-1.5
20125\H,0,-1.540393,0.746325,4.503869\H,0,-1.754419,2.416807,3.934809\
H,0,-3.193407,1.37625,4.163525\H,0,-2.430424,4.3432,-1.931545\H,0,-1.1
71925,4.670297,-0.699757\H,0,-0.689022,4.041804,-2.29084\H,0,-3.254607
, -4.1856,1.039077\H,0,-1.465102,-4.408179,0.934598\H,0,-2.196896,-3.74
0871,2.411239\H,0,-0.636213,-0.849806,-4.494913\H,0,-1.501676,-2.32976
, -4.010063\H,0,-2.437214,-0.927028,-4.597447\Rh,0,-3.004958,0.180002,-
0.215931\H,0,1.97327,0.51414,3.224431\H,0,3.683025,0.282586,2.733004\H
,0,3.191027,1.7613,3.600226\H,0,0.689178,2.568676,2.22344\H,0,2.093539
,3.674542,2.368555\H,0,1.326441,3.384789,0.772773\Version=ES64L-G09Re
vd.01\State=1-A\HF=-2279.3429811\RMSD=2.099e-09\Dipole=-0.6817896,0.12
61017,3.0105255\Quadrupole=-31.7902319,21.5381553,10.2520767,1.1673166
,19.4073886,8.5633752\PG=C01 [X(C20H25N1O11Rh2S1)]\@

M-¹INT5

1\1\GINB-A754\SP\RBPW91\GenECP\C20H25N1O11Rh2S1\SIOC001\15-Mar-2018\0\
\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\Title Card
Required\0,1\C,0,-2.03599,-2.568116,1.595791\H,0,-2.282396,-3.185756
,2.474965\H,0,-1.131242,-2.958965,1.108418\O,0,-3.17822,-2.696952,0.73
6996\O,0,-4.182448,-2.713557,-1.524617\S,0,-2.93597,-2.293449,-0.88188

2\O,0,-1.636682,-2.840306,-1.314721\N,0,-2.997839,-0.596613,-0.897888\
C,0,-2.395712,0.18041,-0.015472\Rh,0,0.498892,0.01524,0.22991\Rh,0,2.7
79307,0.22164,-0.657337\O,0,1.010777,-1.960878,0.631302\O,0,3.123072,-
1.744052,-0.22802\O,0,1.30954,0.610645,2.055388\C,0,2.572449,0.852821,
2.148129\O,0,3.434437,0.764155,1.208387\O,0,0.278311,2.012109,-0.26466
9\O,0,2.405685,2.178637,-1.101429\O,0,-0.052963,-0.424238,-1.705921\C,
0,0.834082,-0.524692,-2.633048\O,0,2.093465,-0.327767,-2.499275\C,0,0.
313746,-0.914598,-3.998852\C,0,3.067792,1.281979,3.515495\C,0,-1.35081
6,-0.284668,0.91616\C,0,2.174519,-2.413206,0.306647\C,0,2.416289,-3.88
2665,0.582383\C,0,1.25023,2.650751,-0.822792\C,0,0.984177,4.104248,-1.
156078\C,0,-2.797278,1.610823,-0.024076\C,0,-2.31978,2.500511,0.96271\
C,0,-3.741739,2.072982,-0.968406\C,0,-2.784645,3.820216,1.011871\H,0,-
1.573806,2.157783,1.684386\C,0,-4.188807,3.396228,-0.927201\H,0,-4.120
093,1.374889,-1.718041\C,0,-3.716464,4.273032,0.065738\H,0,-2.413666,4
.497562,1.786131\H,0,-4.917291,3.744633,-1.664609\H,0,-4.077989,5.3047
4,0.1026\H,0,3.465438,-4.139241,0.386765\H,0,2.158643,-4.121775,1.6255
15\H,0,1.763135,-4.486573,-0.067876\H,0,-0.245655,-1.858783,-3.916593\
H,0,-0.388542,-0.147151,-4.360822\H,0,1.144301,-1.021729,-4.708448\H,0
,0.934317,4.691554,-0.224826\H,0,1.787726,4.501081,-1.789994\H,0,0.012
76,4.203568,-1.661995\H,0,2.890407,0.476773,4.246028\H,0,4.139945,1.51
3735,3.47701\H,0,2.506541,2.165929,3.856316\C,0,-1.796222,-1.098863,2.
116908\C,0,-3.122642,-0.564509,2.722578\C,0,-0.737506,-1.213534,3.2368
08\H,0,-2.993971,0.459545,3.106061\H,0,-3.941656,-0.566626,1.989746\H,
0,-3.421988,-1.206147,3.568565\H,0,0.19965,-1.64901,2.867961\H,0,-0.51
1633,-0.224611,3.658217\H,0,-1.13537,-1.850838,4.044924\\Version=ES64L
-G09RevD.01\State=1-A\HF=-2279.3711864\RMSD=2.493e-09\Dipole=1.0152535
,2.3637691,2.7361988\Quadrupole=-25.3069751,12.7165981,12.5903769,-21.
3624531,-1.9041705,-8.6650998\PG=C01 [X(C20H25N1O11Rh2S1)]\@

M⁻¹INT6

1\1\GINB-A755\SP\RBPW91\GenECP\C20H25N1O11Rh2S1\SIOC001\15-Mar-2018\O\
\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\\Title Card
Required\\0,1\Rh,0,-0.646396,0.169355,0.106665\Rh,0,-2.80342,-0.95049
, -0.195687\O,0,-1.635764,1.933641,-0.388501\C,0,-2.894603,1.894795,-0.
664403\O,0,-3.648763,0.862101,-0.641834\O,0,-1.179737,0.428371,2.08942
2\C,0,-2.315394,-0.02866,2.502071\O,0,-3.182266,-0.643212,1.792625\O,0
,0.120921,-1.703628,0.54402\C,0,-0.644306,-2.73933,0.480676\O,0,-1.897
525,-2.73894,0.21955\O,0,-0.380248,-0.185656,-1.916811\C,0,-1.266905,-
0.819788,-2.599974\O,0,-2.393677,-1.252733,-2.167445\C,0,-3.525692,3.2
08907,-1.081476\C,0,-0.917804,-1.087106,-4.048348\C,0,-2.624075,0.1807
12,3.970365\C,0,0.021864,-4.07159,0.75245\C,0,3.369359,1.439647,2.1812
71\C,0,2.286249,-0.799104,2.612436\C,0,3.095426,0.037072,1.590261\C,0,
2.32436,0.119089,0.242178\N,0,2.589242,-0.550124,-0.846782\S,0,3.82994
5,-1.705834,-0.90691\O,0,4.304459,-1.915371,0.686323\C,0,4.463841,-0.6

29297,1.336023\O,0,3.242036,-2.994351,-1.287003\O,0,4.93821,-1.114698,
-1.675203\C,0,1.152024,1.021268,0.158651\C,0,1.405326,2.427527,-0.1052
42\C,0,2.470727,2.821878,-0.96913\C,0,2.699293,4.171451,-1.245407\C,0,
1.912957,5.161485,-0.629908\C,0,0.87904,4.792622,0.248031\C,0,0.607353
,3.444428,0.490797\H,0,4.967732,-0.848077,2.289974\H,0,5.125701,0.0155
66,0.730395\H,0,3.079948,2.052002,-1.448617\H,0,3.501234,4.455745,-1.9
3232\H,0,2.108251,6.21847,-0.831924\H,0,0.276742,5.56353,0.736917\H,0,
-0.193058,3.15043,1.169708\H,0,-0.667537,-4.895158,0.525559\H,0,0.9370
47,-4.157484,0.147687\H,0,0.316205,-4.128017,1.813251\H,0,-1.798035,-1
.454969,-4.591571\H,0,-0.530597,-0.171936,-4.520126\H,0,-0.118239,-1.8
44401,-4.091162\H,0,-1.949363,-0.441053,4.581048\H,0,-2.448879,1.23094
8,4.248878\H,0,-3.664136,-0.097857,4.183539\H,0,-3.182152,4.024874,-0.
429111\H,0,-3.209762,3.450394,-2.10982\H,0,-4.620523,3.132689,-1.05337
6\H,0,2.828383,-0.807839,3.574331\H,0,1.288945,-0.366096,2.775869\H,0,
2.162124,-1.833277,2.266447\H,0,3.898019,2.096898,1.473426\H,0,2.43772
1,1.940084,2.483417\H,0,3.996729,1.329629,3.082547\\Version=ES64L-G09R
evD.01\State=1-A\HF=-2279.3839759\RMSD=7.372e-09\Dipole=-0.3835046,3.5
728128,2.5180239\Quadrupole=-18.8883967,9.0888815,9.7995152,9.3908725,
12.8034568,-6.6559087\PG=C01 [X(C20H25N1O11Rh2S1)]\@

M-¹TS4

1\1\GINB-A755\SP\RBPW91\GenECP\C20H25N1O11Rh2S1\SI0C001\15-Mar-2018\O\
\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\\Title Card
Required\\0,1\O,0,-3.014793,-2.553062,0.979862\O,0,-4.782931,-2.51552
2,-0.80945\S,0,-3.344122,-2.252581,-0.737836\O,0,-2.386643,-3.059414,-
1.507301\N,0,-3.110756,-0.625621,-0.892621\C,0,-2.44346,0.129905,-0.03
0902\Rh,0,0.54634,-0.05022,0.192432\Rh,0,2.836952,0.164664,-0.646432\O
,0,0.247144,-1.471617,-1.25225\O,0,2.379356,-1.243897,-2.066329\O,0,1.
285132,-1.584564,1.414095\C,0,2.540958,-1.885142,1.364023\O,0,3.425875
, -1.318781,0.638974\O,0,1.046195,1.389921,1.613912\O,0,3.18601,1.57953
4,0.801203\O,0,0.057903,1.433939,-1.159567\C,0,0.967979,1.93772,-1.918
909\O,0,2.21085,1.630368,-1.923514\C,0,0.504696,2.978424,-2.918367\C,0
,2.989473,-3.038879,2.241207\C,0,-1.442942,-0.275183,0.979938\C,0,-1.7
51971,-2.194536,1.341958\C,0,1.206869,-1.760318,-2.065321\C,0,0.908903
, -2.814136,-3.1115\C,0,2.240124,1.880368,1.607934\C,0,2.56118,2.888488
,2.696196\C,0,-2.725343,1.590266,-0.128486\C,0,-2.022972,2.537544,0.65
1183\C,0,-3.774236,2.037701,-0.96505\C,0,-2.373646,3.892242,0.60393\H,
0,-1.174743,2.222939,1.263088\C,0,-4.109438,3.393627,-1.01905\H,0,-4.3
22983,1.303983,-1.55832\C,0,-3.414447,4.326666,-0.231447\H,0,-1.819373
,4.61392,1.210732\H,0,-4.922831,3.723385,-1.671382\H,0,-3.682422,5.386
508,-0.269863\H,0,1.113372,-2.405176,-4.113296\H,0,1.58065,-3.675461,-
2.966494\H,0,-0.135984,-3.140215,-3.042278\H,0,0.034152,2.470752,-3.77
6765\H,0,-0.250087,3.635549,-2.463986\H,0,1.359344,3.565055,-3.281039\
H,0,1.666837,3.465876,2.969446\H,0,2.910393,2.352787,3.595186\H,0,3.36

4624,3.561236,2.366618\H,0,2.566291,-2.942099,3.252459\H,0,2.620093,-3.9868,1.815767\H,0,4.085373,-3.07616,2.293216\C,0,-1.82394,-0.42166,2.333378\C,0,-3.257076,-0.24176,2.792682\C,0,-0.813012,-0.488266,3.454732\H,0,-1.490292,-2.618379,2.318862\H,0,-0.957599,-2.390165,0.605598\H,0,-3.359975,0.790262,3.173387\H,0,-3.990677,-0.379304,1.988452\H,0,-3.500971,-0.922825,3.623896\H,0,0.171221,-0.820683,3.10685\H,0,-0.699374,0.532156,3.860321\H,0,-1.170964,-1.130119,4.277387\\Version=ES64L-G09 RevD.01\State=1-A\HF=-2279.3493627\RMSD=5.328e-09\Dipole=0.1204716,1.741988,3.3376667\Quadrupole=-27.8433788,10.3714408,17.471938,-21.3081928,-3.1112012,-7.5086451\PG=C01 [X(C20H25N1O11Rh2S1)]\@

M-1TS5

1\1\GINB-A754\SP\RBPW91\GenECP\C20H25N1O11Rh2S1\SI0C001\15-Mar-2018\0\
\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\\Title Card
Required\\0,1\C,0,-3.07024,-2.33679,1.78511\H,0,-3.592104,-2.254657,2.754092\H,0,-2.788272,-3.396888,1.651016\O,0,-4.023307,-1.949268,0.805152\O,0,-4.531112,-2.225498,-1.65489\S,0,-3.372723,-1.991899,-0.789319\O,0,-2.235519,-2.937958,-0.777363\N,0,-2.97678,-0.377752,-0.955981\C,0,-2.413959,0.255292,0.069539\Rh,0,0.556529,-0.020837,0.212095\Rh,0,2.835416,0.128039,-0.679406\O,0,0.796021,-2.079122,0.046769\O,0,2.928499,-1.909876,-0.776248\O,0,1.413325,0.00674,2.113038\C,0,2.700394,0.076515,2.219673\O,0,3.538439,0.111946,1.257922\O,0,0.596721,2.053447,0.238852\O,0,2.718168,2.167436,-0.615331\O,0,-0.075537,0.004974,-1.749473\C,0,0.788754,0.075504,-2.699473\O,0,2.062795,0.155395,-2.567669\C,0,0.23241,0.040606,-4.107828\C,0,3.254139,0.133895,3.631113\C,0,-1.469265,-0.391597,1.021456\C,0,1.889746,-2.569404,-0.418611\C,0,1.949785,-4.080387,-0.535884\C,0,1.635998,2.689711,-0.176879\C,0,1.573356,4.203554,-0.113117\C,0,-2.70705,1.719723,0.095558\C,0,-2.06544,2.655055,0.942445\C,0,-3.771361,2.184949,-0.719388\C,0,-2.48175,3.992587,0.979886\H,0,-1.205411,2.357721,1.537447\C,0,-4.169683,3.523535,-0.693178\H,0,-4.284658,1.466731,-1.360418\C,0,-3.53249,4.435317,0.164054\H,0,-1.970518,4.693711,1.645848\H,0,-4.993537,3.853011,-1.332362\H,0,-3.854819,5.480033,0.197987\H,0,2.013195,-4.529359,0.469321\H,0,1.031449,-4.454816,-1.012024\H,0,2.830546,-4.383928,-1.116752\H,0,-0.627239,0.721613,-4.191005\H,0,1.009212,0.312479,-4.834435\H,0,-0.131066,-0.976393,-4.328233\H,0,0.560386,4.554727,-0.354854\H,0,1.815449,4.537609,0.909932\H,0,2.306477,4.642195,-0.803301\H,0,4.349096,0.059361,3.614811\H,0,2.963269,1.086382,4.103699\H,0,2.832898,-0.680091,4.241162\C,0,-1.74603,0.050941,2.739663\C,0,-1.748712,-1.556109,1.795379\C,0,-0.673672,-2.359113,2.500664\H,0,-2.418886,0.890686,2.530456\H,0,-0.746079,0.333755,3.084332\H,0,-0.405322,-3.192909,1.836075\H,0,-1.06346,-2.774729,3.44683\H,0,0.230696,-1.769799,2.686597\H,0,-2.255338,-0.534314,3.526517\\Version=ES64L-G09 RevD.01\State=1-A\HF=-2279.3298424\RMSD=7.643e-09\Dipole=0.3239723,1.2846579,4.4736459\Quadrupole=-30.6656766,13.668018,16.9976587,-14.14

10197,-9.889326,-9.5369372\PG=C01 [X(C20H25N1O11Rh2S1)]\@

M-¹INT5.H2O

1\1\GINB-OM103\SP\RBPW91\GenECP\C20H27N1O12Rh2S1\WEIY\27-Apr-2018\0\#\#
p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\Title Card R
equired\0,1\C,0,-2.728377,-2.041295,2.082929\H,0,-3.694217,-1.721464,
1.652489\H,0,-2.937444,-2.510601,3.060133\O,0,-2.127536,-3.113089,1.29
2148\O,0,-3.857781,-3.52357,-0.96728\S,0,-2.448353,-2.810585,-0.584175
\O,0,-1.109226,-3.315972,-1.363703\N,0,-2.958809,-0.91776,-0.754153\C,
0,-2.426754,0.030098,0.000476\Rh,0,0.485961,0.077327,0.240576\Rh,0,2.6
91408,0.146148,-0.884006\O,0,0.9191,-1.914885,0.584309\O,0,2.950283,-1
.849177,-0.533336\O,0,1.520854,0.588068,2.001792\C,0,2.83616,0.727196,
1.979441\O,0,3.569864,0.590668,0.917855\O,0,0.348848,2.123608,-0.17369
1\O,0,2.385558,2.138183,-1.28039\O,0,-0.273604,-0.331191,-1.642517\C,0
,0.515041,-0.500901,-2.681498\O,0,1.808065,-0.337344,-2.660828\C,0,-0.
140857,-0.929322,-3.963516\C,0,3.506734,1.072914,3.282967\C,0,-1.3427,
-0.191891,0.997239\C,0,2.003653,-2.481605,0.106187\C,0,2.133413,-3.964
576,0.309025\C,0,1.303594,2.724026,-0.866365\C,0,1.118798,4.190594,-1.
151027\C,0,-2.973279,1.394653,-0.292641\C,0,-2.747937,2.48027,0.584492
\C,0,-3.759687,1.592485,-1.457075\C,0,-3.309181,3.738196,0.304907\H,0,
-2.133951,2.356109,1.477332\C,0,-4.312702,2.850053,-1.728704\H,0,-3.92
5044,0.752579,-2.132495\C,0,-4.091788,3.92809,-0.847252\H,0,-3.131317,
4.566998,0.99339\H,0,-4.915508,2.991905,-2.628258\H,0,-4.526817,4.9073
24,-1.060109\H,0,3.125797,-4.304117,-0.011625\H,0,1.965628,-4.22219,1.
365502\H,0,1.352587,-4.471367,-0.280432\H,0,0.590316,-0.924269,-4.7809
54\H,0,-0.547025,-1.944836,-3.829314\H,0,-0.983323,-0.263382,-4.202731
\H,0,0.082337,4.390526,-1.457632\H,0,1.318687,4.776767,-0.237881\H,0,1
.818033,4.50955,-1.933819\H,0,4.589351,1.163446,3.13407\H,0,3.1073,2.0
22345,3.674552\H,0,3.299881,0.29231,4.03212\C,0,-1.766809,-0.827298,2.
328579\C,0,-2.612797,0.228289,3.132934\C,0,-0.588027,-1.304969,3.20797
3\H,0,-3.508447,0.551697,2.58046\H,0,-2.001273,1.110034,3.374163\H,0,-
0.03771,-2.107809,2.702226\H,0,-0.988355,-1.688655,4.161838\O,0,-0.155
504,2.782099,2.585298\H,0,0.395651,1.98203,2.778782\H,0,-0.114248,2.86
4754,1.598173\H,0,0.108325,-0.485686,3.423326\H,0,-2.935846,-0.245903,
4.075256\Version=ES64L-G16RevA.03\State=1-A\HF=-2355.7532999\RMSD=7.7
33e-09\Dipole=0.4531759,3.080399,1.5285552\Quadrupole=-8.9852455,-3.82
53809,12.8106264,-21.0368548,4.281439,-15.2797739\PG=C01 [X(C20H27N1O1
2Rh2S1)]\@

M-¹TS6

1\1\GINB-A759\SP\RBPW91\GenECP\C20H27N1O12Rh2S1\SIOC001\24-Mar-2018\0\
\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\Title Card
Required\0,1\C,0,-3.313014,-1.653085,1.852235\H,0,-3.897371,-0.72255
7,1.73537\H,0,-3.626247,-2.126381,2.799648\O,0,-3.736516,-2.672135,0.8

82914\O,0,-4.874685,-2.218647,-1.679125\S,0,-3.42541,-2.190866,-0.9489
08\O,0,-2.261275,-3.17315,-1.537837\N,0,-3.103608,-0.237493,-0.874747\
C,0,-2.357134,0.365801,0.033143\Rh,0,0.62274,-0.051493,0.191983\Rh,0,2
.932084,0.13839,-0.698536\O,0,0.560839,-1.869042,-0.754652\O,0,2.71280
9,-1.681632,-1.602988\O,0,1.496566,-0.884253,1.897796\C,0,2.797179,-1.
081738,1.946617\O,0,3.63896,-0.767654,1.002059\O,0,0.9732,1.821993,1.0
86992\O,0,3.114917,1.968808,0.237947\O,0,-0.006182,0.805938,-1.592566\
C,0,0.874169,1.137878,-2.514439\O,0,2.166262,1.02105,-2.386473\C,0,0.3
2925,1.672586,-3.812676\C,0,3.340545,-1.749269,3.18484\C,0,-1.326686,-
0.218827,0.948885\C,0,1.575923,-2.310235,-1.46074\C,0,1.405868,-3.6521
19,-2.118991\C,0,2.14876,2.426835,0.963234\C,0,2.346234,3.712493,1.722
854\C,0,-2.72634,1.84197,-0.041672\C,0,-1.799281,2.884098,-0.293888\C,
0,-4.102942,2.162753,0.089107\C,0,-2.245397,4.213569,-0.392599\H,0,-0.
749556,2.640301,-0.435109\C,0,-4.536687,3.495011,-0.004982\H,0,-4.8232
83,1.359194,0.247581\C,0,-3.610132,4.525014,-0.247041\H,0,-1.52287,5.0
06486,-0.599165\H,0,-5.599155,3.723253,0.099496\H,0,-3.948535,5.560064
, -0.328732\H,0,2.048914,-3.71974,-3.00639\H,0,1.702341,-4.448379,-1.41
4988\H,0,0.351537,-3.806668,-2.383084\H,0,-0.49158,2.378784,-3.62285\H
,0,1.129126,2.155851,-4.387461\H,0,-0.084275,0.839178,-4.404911\H,0,3.
295277,4.176904,1.429251\H,0,1.514377,4.407277,1.530594\H,0,2.364991,3
.508429,2.806484\H,0,3.153854,-2.835196,3.131454\H,0,4.422519,-1.58242
4,3.258638\H,0,2.831957,-1.366631,4.081104\C,0,-1.776191,-1.376394,1.9
19154\C,0,-1.450041,-1.03726,3.410609\C,0,-1.026466,-2.709849,1.599007
\H,0,-2.086871,-0.233992,3.802043\H,0,-0.400878,-0.733447,3.508049\H,0
, -1.098956,-3.002033,0.546447\H,0,-1.487629,-3.504465,2.208954\O,0,-1.
272797,1.404717,2.313957\H,0,-0.333209,1.688842,2.05893\H,0,-1.90305,2
.063857,1.927842\H,0,-1.609684,-1.955193,4.001532\H,0,0.030537,-2.6086
81,1.869815\\Version=ES64L-G09RevD.01\State=1-A\HF=-2355.7295217\RMSE=
5.432e-09\Dipole=1.4912627,4.2205401,3.1433025\Quadrupole=-24.5334984,
15.9191704,8.6143281,-27.7296125,-8.4070747,-6.9554676\PG=C01 [X(C20H2
7N1O12Rh2S1)]\@

M-1INT6.H2O

1\1\GINB-A750\SP\RBPW91\GenECP\C20H27N1O12Rh2S1\SI0C001\15-Mar-2018\O\
\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\\Title Card
Required\\0,1\Rh,0,-0.697744,0.084788,0.197295\Rh,0,-2.925085,-0.8225
81,-0.289257\O,0,-1.152507,1.549075,-1.214219\C,0,-2.306001,1.547226,-
1.803131\O,0,-3.249537,0.711195,-1.601692\O,0,-1.615326,1.20315,1.6949
42\C,0,-2.882441,1.063935,1.903446\O,0,-3.676325,0.308936,1.246491\O,0
, -0.502878,-1.469859,1.541904\C,0,-1.437631,-2.354596,1.640279\O,0,-2.
55352,-2.347682,1.01714\O,0,-0.045496,-1.177341,-1.292006\C,0,-0.87727
8,-1.87189,-1.990478\O,0,-2.144478,-1.934105,-1.809381\C,0,-2.524215,2
.632636,-2.834814\C,0,-0.272721,-2.651928,-3.134008\C,0,-3.461349,1.86
7215,3.050433\C,0,-1.166715,-3.513408,2.576998\C,0,3.115898,1.01483,2.

652137\C,0,2.371165,-1.390431,2.61404\C,0,3.059943,-0.270637,1.79683\C,0,2.319338,-0.039726,0.448956\N,0,2.662519,-0.551152,-0.704485\S,0,3.990906,-1.599895,-0.883283\O,0,4.514429,-1.908134,0.674747\C,0,4.507344,-0.697257,1.473683\O,0,3.508286,-2.892062,-1.378139\O,0,5.021921,-0.833964,-1.600769\C,0,1.145336,0.866451,0.390317\C,0,1.431038,2.281211,0.229206\C,0,2.675107,2.727103,-0.319122\C,0,2.938164,4.086044,-0.486236\C,0,1.987722,5.043474,-0.08857\C,0,0.760446,4.630171,0.457998\C,0,0.472381,3.271374,0.596974\H,0,5.046735,-0.960415,2.396272\H,0,5.069407,0.099811,0.95434\H,0,3.40805,1.992119,-0.656935\H,0,3.885356,4.40384,-0.929983\H,0,2.202532,6.109061,-0.209615\H,0,0.023206,5.375377,0.769714\H,0,-0.474148,2.945007,1.026899\H,0,-2.082661,-4.098569,2.730304\H,0,-0.391824,-4.16274,2.138069\H,0,-0.785882,-3.145782,3.541429\H,0,-1.013314,-3.335587,-3.568881\H,0,0.070882,-1.936571,-3.899187\H,0,0.61095,-3.206083,-2.784607\H,0,-3.073261,1.475839,4.004885\H,0,-3.148771,2.919734,2.974416\H,0,-4.556811,1.798812,3.049151\H,0,-2.196817,3.605695,-2.439581\H,0,-1.911151,2.413766,-3.724641\H,0,-3.581471,2.674087,-3.126858\H,0,2.936111,-1.543755,3.55009\H,0,1.338451,-1.116029,2.860828\H,0,2.352817,-2.339029,2.059744\H,0,3.610093,1.848975,2.130746\H,0,2.106746,1.344573,2.943098\H,0,3.679115,0.804878,3.577124\O,0,1.174302,0.99457,-3.058124\H,0,1.598723,0.306061,-2.502464\H,0,0.447968,1.303025,-2.478937\\Version=ES64L-G09RevD.01\State=1-A\HF=-2355.8432698\RMSE=4.559e-09\Dipole=-0.8823459,2.9003643,3.8305434\Quadrupole=-16.9460712,15.4223832,1.523688,7.56725,17.04916,-3.5795772\PG=C01 [X(C20H27N1O12Rh2S1)]\@

M-1TS7

1\1\GINB-A764\SP\RBPW91\GenECP\C20H27N1O12Rh2S1\SI0C001\15-Mar-2018\0\ \#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\Title Card Required\0,1\Rh,0,-0.646905,0.100838,-0.053986\Rh,0,-2.881904,-0.899446,0.194594\O,0,-1.619568,1.740565,-0.882104\C,0,-2.905112,1.73646,-0.98037\O,0,-3.696624,0.797966,-0.616858\O,0,-0.915425,0.866302,1.85416\C,0,-2.008106,0.608395,2.494431\O,0,-2.995009,-0.075767,2.060913\O,0,0.100456,-1.66198,0.721012\C,0,-0.71112,-2.611197,1.041866\O,0,-1.989607,-2.574838,0.9672\O,0,-0.679935,-0.77999,-1.942548\C,0,-1.687024,-1.486937,-2.349844\O,0,-2.7393,-1.72218,-1.674614\C,0,-3.53158,2.986754,-1.566992\C,0,-1.571256,-2.085999,-3.734366\C,0,-2.099454,1.15783,3.903937\C,0,-0.073153,-3.877486,1.57475\C,0,3.536392,1.726438,1.647267\C,0,2.196996,-0.227211,2.511099\C,0,3.090404,0.273613,1.351785\C,0,2.378111,0.119146,-0.032422\N,0,2.709252,-0.806698,-0.906442\S,0,3.789904,-2.077422,-0.634363\O,0,4.146291,-1.94431,0.985169\C,0,4.395338,-0.555914,1.320258\O,0,3.066081,-3.344923,-0.767867\O,0,4.990908,-1.803623,-1.438691\C,0,1.224118,0.99149,-0.393427\C,0,1.397008,2.462143,-0.421687\C,0,2.449364,3.061735,-1.164328\C,0,2.626872,4.446762,-1.169103\C,0,1.776655,5.270836,-0.410478\C,0,0.740214,4.695034,0.33733\C,0,0.53633,3

.308197,0.318008\H,0,4.843337,-0.582622,2.324512\H,0,5.134632,-0.130756,0.618235\H,0,3.105597,2.427617,-1.763397\H,0,3.4337,4.887425,-1.76162\H,0,1.921984,6.354921,-0.407284\H,0,0.075549,5.328741,0.931707\H,0,-0.267335,2.863517,0.902986\H,0,-3.136839,1.119975,4.261173\H,0,-1.470346,0.547853,4.573399\H,0,-1.720691,2.189855,3.940351\H,0,0.835973,-4.109569,1.001797\H,0,0.220475,-3.72473,2.626917\H,0,-0.785733,-4.711601,1.527348\H,0,-3.51726,3.790383,-0.812144\H,0,-2.94878,3.334412,-2.432351\H,0,-4.572215,2.792523,-1.858269\H,0,-2.502696,-2.59992,-4.003935\H,0,-1.352721,-1.298955,-4.473108\H,0,-0.735159,-2.803425,-3.756646\O,0,1.408789,0.7173,-2.477614\H,0,2.00004,-0.079259,-2.300854\H,0,0.517959,0.287399,-2.582437\H,0,2.741784,-0.085459,3.461053\H,0,1.254906,0.335472,2.55931\H,0,1.957584,-1.291565,2.394625\H,0,4.124207,2.162988,0.825686\H,0,2.682756,2.386503,1.847399\H,0,4.170031,1.714591,2.551527\\Version=ES64L-G09RevD.01\State=1-A\HF=-2355.8289581\RMSD=8.923e-09\Dipole=-0.2113114,3.0874197,1.5671751\Quadrupole=-16.7413846,3.3298247,13.4115599,11.3387732,14.8993571,1.1258786\PG=C01 [X(C20H27N1O12Rh2S1)]\@

M-INT7

1\1\GINB-A761\SP\RBPW91\GenECP\C20H27N1O12Rh2S1\SIOC001\15-Mar-2018\0\#p genecp scrf=(iefpcm,smd,solvent=dichloromethane) bpw91\Title Card Required\0,1\Rh,0,-0.501052,0.18979,-0.003336\Rh,0,-2.912053,-0.019913,0.148526\O,0,-0.835563,1.68805,-1.420293\C,0,-2.0502,2.018937,-1.71728\O,0,-3.105368,1.510955,-1.207627\O,0,-0.635027,1.525183,1.577761\C,0,-1.790641,1.807658,2.071037\O,0,-2.915618,1.331422,1.685003\O,0,-0.385922,-1.322309,1.380179\C,0,-1.46674,-1.879621,1.801663\O,0,-2.663927,-1.54886,1.478596\O,0,-0.600163,-1.167632,-1.562651\C,0,-1.736467,-1.675886,-1.894715\O,0,-2.870794,-1.382889,-1.374415\C,0,-2.218047,3.107259,-2.757296\C,0,-1.715056,-2.720275,-2.989681\C,0,-1.81399,2.803957,3.213432\C,0,-1.297329,-3.036878,2.76133\C,0,4.499244,0.29839,0.882903\C,0,2.494098,-0.249919,2.344782\C,0,3.2204,-0.572962,1.020212\C,0,2.313378,-0.436724,-0.227477\N,0,2.223762,-1.572963,-1.043016\S,0,2.088921,-3.209746,-0.499637\O,0,2.648917,-2.990232,1.028613\C,0,3.741299,-2.027479,1.082464\O,0,0.712482,-3.700268,-0.356517\O,0,3.045045,-3.964408,-1.32207\C,0,1.874893,0.756361,-0.834476\C,0,2.332972,2.147169,-0.499711\C,0,3.168674,2.782843,-1.451526\C,0,3.677258,4.065735,-1.219741\C,0,3.351725,4.752701,-0.03929\C,0,2.501636,4.14541,0.895351\C,0,1.990438,2.858111,0.668141\H,0,4.226523,-2.215334,2.050984\H,0,4.461771,-2.246335,0.276486\H,0,3.426798,2.250035,-2.369418\H,0,4.33369,4.528591,-1.96253\H,0,3.748663,5.755313,0.143841\H,0,2.21951,4.680489,1.807186\H,0,1.28407,2.424344,1.375073\H,0,-2.839056,2.943011,3.580284\H,0,-1.170677,2.448726,4.033638\H,0,-1.411435,3.770745,2.871319\H,0,-0.736242,-3.839043,2.257729\H,0,-0.708755,-2.717939,3.63568\H,0,-2.27613,-3.411206,3.087894\H,0,-1.676298,4.012545,-2.441418\H,0,-1.781371,2.779558,-3.714651\H,0,-3.280776,3.339532,-2.902123\H,0,-2.736903,-2.979218,-3.29

5635\H,0,-1.145018,-2.350712,-3.856099\H,0,-1.203414,-3.620421,-2.6132
43\O,0,1.551447,0.610809,-2.190216\H,0,0.738788,1.159468,-2.328699\H,0
,1.648571,-1.406155,-1.882002\H,0,3.192899,-0.392877,3.187557\H,0,2.15
0466,0.791649,2.363882\H,0,1.621265,-0.900876,2.482901\H,0,4.988839,0.
149511,-0.092987\H,0,4.279134,1.366676,1.001215\H,0,5.216384,0.014846,
1.673241\\Version=ES64L-G09RevD.01\State=1-A\HF=-2355.8617496\RMSD=3.7
39e-09\Dipole=1.2067082,2.4171998,0.7448772\Quadrupole=-5.6978401,-6.3
167609,12.014601,6.6195088,9.5745903,-4.5290461\PG=C01 [X(C20H27N1O12R
h2S1)]\@

M-INT8

1\1\GINC-OM113\SP\RBPW91\GenECP\C20H27N1O12Rh2S1\WEIY\11-Jan-2019\0\#\#
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,0,-3.9559884515,-0.8164184722,1.8329563132\H,0,-3.6279457025,-2.34674
13844,2.6816483138\O,0,-3.6948897924,-2.5639550456,0.7024987381\O,0,-4
.7532384039,-2.1798726,-1.527938185\S,0,-3.4577431974,-1.9881271837,-0
.8670961508\O,0,-2.2560122116,-2.6325375087,-1.4262199616\N,0,-3.26469
89379,-0.3227995743,-0.7148594438\C,0,-2.4538219055,0.3379624996,0.082
7302931\Rh,0,0.6517642585,-0.1065532249,0.0700478927\Rh,0,2.9513466666
,0.1293138833,-0.7440998001\O,0,0.6430229558,-1.9369058405,-0.82878862
68\O,0,2.7688969938,-1.6791839822,-1.657083984\O,0,1.495631511,-0.8734
345698,1.8166408612\C,0,2.7694708351,-1.067826882,1.872101482\O,0,3.62
36887401,-0.7807626756,0.9629526413\O,0,0.9203608734,1.7798943453,0.95
5927567\O,0,3.0717246226,1.9516201982,0.2399690956\O,0,0.0499795129,0.
7044127414,-1.7353218364\C,0,0.9420243713,1.0644601737,-2.5938505947\O
,0,2.2132551744,1.0071727177,-2.440244738\C,0,0.4229350397,1.580694165
7,-3.9203421987\C,0,3.297278655,-1.7254245137,3.1328148668\C,0,-1.4258
571241,-0.1550975969,1.0335897457\C,0,1.6675851409,-2.3234062996,-1.50
16891281\C,0,1.563164043,-3.6881378925,-2.148861584\C,0,2.0844184104,2
.3727932517,0.9094389084\C,0,2.2278848678,3.6487163274,1.7091438651\C,
0,-2.7701385003,1.8245596318,-0.0086310227\C,0,-1.8396307464,2.8242711
497,-0.3774084104\C,0,-4.1083374307,2.2077839256,0.2556666499\C,0,-2.2
421450163,4.1653968967,-0.4724097429\H,0,-0.8198224697,2.5344817996,-0
.6280718021\C,0,-4.4976002463,3.549705711,0.1741901089\H,0,-4.83965888
38,1.4354109912,0.5043418459\C,0,-3.5656508643,4.5335960382,-0.1922328
643\H,0,-1.5166725338,4.9224553926,-0.7837426337\H,0,-5.5348168062,3.8
242707084,0.3842293151\H,0,-3.8726656692,5.580464476,-0.2663234983\H,0
,2.2081216368,-3.7378052422,-3.036973683\H,0,1.9025571768,-4.455394402
3,-1.4327511399\H,0,0.5183834112,-3.9014706093,-2.4117601722\H,0,-0.48
39284955,2.1841675195,-3.7723828925\H,0,1.1974643757,2.1643139825,-4.4
357146668\H,0,0.1483994769,0.7208071099,-4.5538015128\H,0,3.1953366072
,4.1214935098,1.4979793757\H,0,1.4106358766,4.3465750691,1.4689148116\
H,0,2.1646077851,3.4217882419,2.7864655923\H,0,3.0858192082,-2.8070804
615,3.0942391222\H,0,4.3827642766,-1.5816023493,3.2142777264\H,0,2.790

8305618,-1.3192229283,4.020618555\C,0,-1.8185051787,-1.3926774991,1.94
72689266\C,0,-1.5782107913,-1.0786283115,3.4487563228\C,0,-1.020595914
, -2.676660962,1.6156232174\H,0,-2.246871967,-0.2963628378,3.842180571\
H,0,-0.5380106939,-0.7686761738,3.6198645997\H,0,-1.0476181761,-2.9194
642553,0.5483789639\H,0,-1.4651355288,-3.5194292664,2.1726979371\O,0,-
1.2302274564,1.0988032418,2.0540826417\H,0,-0.2976358923,1.4879120755,
1.817964927\H,0,-1.8679359849,1.7982178501,1.7277226332\H,0,-1.7548075
742,-2.0014150921,4.0255876434\H,0,0.0250241829,-2.56151867,1.92471598
53\Version=ES64L-G09RevE.01\State=1-A\HF=-2355.8000793\RMSD=3.986e-09
\Dipole=1.0582344,4.0695513,3.7295432\Quadrupole=-25.4330067,15.725316
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2S1)]\@

M-1PC3

1\1\GINC-OM113\SP\RBPW91\GenECP\C20H25N1O11Rh2S1\WEIY\12-Feb-2019\0\#\#
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16707,-0.1770371457\O,0,-0.9970960101,-2.1721908805,-1.5416813752\O,0,
-0.5797773644,-2.0358356605,-4.0015774741\S,0,-0.4815101449,-1.1932973
719,-2.8081511409\O,0,0.7983158915,-0.5507623723,-2.4360545855\N,0,-1.
7921995402,-0.1251789281,-2.8804896454\C,0,-2.1557485013,0.555417151,-
1.8182512905\Rh,0,-0.6395410958,4.1004241519,-6.3179802569\Rh,0,1.0820
405895,3.2928900604,-7.7495297595\O,0,0.4781551188,3.5075895264,-4.706
1430527\O,0,2.1350217857,2.7305427182,-6.0854243454\O,0,0.2934718507,5
.9293634087,-6.2986889514\C,0,1.378802634,6.0644424041,-6.9762249463\O
,0,1.956483772,5.1498464828,-7.6711027929\O,0,-1.6944243944,4.66562416
85,-7.9889211368\O,0,-0.033812228,3.8886883622,-9.3651940478\O,0,-1.51
11694821,2.2449799978,-6.3994368764\C,0,-0.9323309332,1.3251394275,-7.
0937849143\O,0,0.1525010699,1.4693485419,-7.7695794438\C,0,-1.57161316
99,-0.0437841433,-7.0933253287\C,0,2.0172707179,7.437652832,-6.9804035
611\C,0,-1.4979850509,0.6689206569,-0.4827139542\C,0,1.6177254673,2.94
91589411,-4.9283828873\C,0,2.4035931056,2.4875049793,-3.722476684\C,0,
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, -10.3504713218\C,0,-3.4026449009,1.3511127403,-2.0409577609\C,0,-3.66
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0186784981\C,0,-4.8569935154,2.6228919826,-3.5251511497\H,0,-2.9196452
756,1.8324455626,-4.0985460299\C,0,-5.5726607583,2.1420064586,-1.25295
30914\H,0,-4.1904887185,0.9925575922,-0.0486543051\C,0,-5.8150399063,2
.7308746765,-2.503656599\H,0,-5.041408664,3.0785967059,-4.5019525501\H
,0,-6.3217038031,2.2082005727,-0.4589994206\H,0,-6.7494809973,3.270164
539,-2.6827768735\H,0,2.2989308205,3.2138746687,-2.9033870156\H,0,2.00
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842588093\H,0,-2.6669739426,0.0491322852,-7.1193622923\H,0,-1.21644981
09,-0.6309542279,-7.9505988891\H,0,-1.301815236,-0.5744154194,-6.16523

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5.9907097425,-10.5082860036\H,0,-1.6401238756,4.3704873213,-11.2501740
316\H,0,3.0947700028,7.3588850718,-7.1788541829\H,0,1.5613578979,8.045
7528233,-7.7797538011\H,0,1.837744034,7.9456387777,-6.0226174547\C,0,-
1.5381211058,2.061844821,0.1434026127\C,0,-0.8267045566,-0.3233277685,
0.1804136404\C,0,-0.2091207789,-0.0469837528,1.5378115412\H,0,-1.91557
83235,2.8117496637,-0.563507071\H,0,-0.522458943,2.370975228,0.4414343
78\H,0,0.6811793724,0.6001307659,1.4368036261\H,0,0.1168397801,-0.9755
728111,2.0327622503\H,0,-0.9096603187,0.4694694057,2.2132181625\H,0,-2
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M-¹PC4

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,2.3399036457\O,0,2.252510645,-0.0172058989,2.5850014448\N,0,0.7689372
13,-1.9587867267,1.91074418\C,0,0.4190547608,-2.3499626319,0.706150708
5\Rh,0,3.4898867127,-1.2148783086,-3.1314142156\Rh,0,5.6716990025,-1.1
782729715,-4.0770008935\O,0,4.101109111,0.2278137006,-1.8073647869\O,0
,6.2034727449,0.256180502,-2.7162989206\O,0,2.9319136703,0.2441645992,
-4.4650904214\C,0,3.8165441025,0.6795660493,-5.2926510924\O,0,5.033835
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994\O,0,5.0603339082,-2.6223327205,-5.4035924157\O,0,4.1301296784,-2.6
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0,0.1072427756,-4.6785137408,1.5922757094\C,0,1.0001254659,-5.79126810
17,-0.8238923505\H,0,1.2089014024,-3.7513196718,-1.5165165751\C,0,0.18
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5311666185\C,0,0.6337869981,-6.6286237585,0.2411425788\H,0,1.364956810
5,-6.22135825,-1.7609663803\H,0,-0.099130708,-6.7156272029,2.282396128
9\H,0,0.6999770092,-7.7149674939,0.132632176\H,0,6.8054090856,1.873541
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076225\H,0,4.9932082887,-4.7645703636,-0.6428975189\H,0,6.693273689,-4
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59179,-6.6124503312\H,0,2.3463042006,1.6408135945,-6.5453513262\H,0,3.
453446856,2.7532060488,-5.7059336047\H,0,4.0518683352,1.8229764053,-7.
1085508952\C,0,-0.803269295,-1.6323781429,-1.3959997434\C,0,-1.7711226
588,-2.7937314937,-1.4250012769\C,0,-1.0336695962,-0.6645777857,-2.538
0237068\H,0,0.6518102986,0.6350732869,-1.0235671282\H,0,1.948082178,-0
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8\H,0,-1.7908364745,-3.3824198718,-0.5010690326\H,0,-2.78766728,-2.400
6848183,-1.6077387251\H,0,-0.2098657624,0.0388381515,-2.7152961844\H,0
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[X(C20H25N1O11Rh2S1)]\@

Mf-¹INT4

1\1\GINB-A758\SP\RBPW91\GenECP\C44H53N1O11Rh2S1\SI0C001\20-Mar-2018\0\
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280466\O,0,-1.315032,0.615781,-1.260924\O,0,1.857986,-0.886106,-2.2076
67\C,0,2.16157,0.304101,-1.837266\O,0,1.598382,0.953963,-0.878615\O,0,
1.808697,-2.610709,0.154234\C,0,2.127355,-1.868187,1.148603\O,0,1.5874
34,-0.734506,1.434959\O,0,-1.044711,-2.930183,-0.190027\C,0,-1.655428,
-2.323054,0.758311\O,0,-1.397466,-1.129653,1.167242\C,0,-2.572022,0.37
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1934\H,0,-3.891256,-1.307972,2.070263\C,0,-2.33097,-3.316709,2.959234\
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-1.396741,-3.900599,3.004595\C,0,-2.007858,1.68111,-3.933512\H,0,-2.73
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,1.482828,-4.480734\C,0,-3.919696,0.721708,-2.579604\H,0,-3.723811,1.5
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57,-1.803048,0.462844\C,0,6.270866,-1.107018,0.959617\C,0,4.645131,-1.
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,1.925623\C,0,5.170922,-0.361193,-1.533422\H,0,3.805935,-1.999064,-1.2
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Mf⁻¹TS2

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Mf-1TS3

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,0,-2.195669,-0.773584,1.804462\0,0,-1.643423,0.258753,1.275886\0,0,-1
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34508,-0.074518,-1.62624\0,0,1.177646,-2.690733,-1.052472\C,0,1.786542
,-1.696412,-1.580575\0,0,1.485288,-0.456234,-1.395532\C,0,2.510579,-1.
147588,3.28889\C,0,2.962141,-2.005937,-2.537685\C,0,2.795737,-2.57732,
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Mf-¹INT5

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, -0.179256,-2.366485\C,-2.355585,0.848803,-1.66013\O,-1.776353,1.1882,
-0.561208\O,0.765631,-0.312846,-2.799912\C,1.365568,0.662815,-2.225791
\O,1.161952,1.050554,-1.012578\C,2.712789,-3.253404,0.435359\C,2.39237
7,1.458,-3.065633\C,2.965034,-4.337867,-0.630738\H,3.765174,-5.011556,
-0.279609\H,2.061373,-4.939704,-0.809188\C,3.732767,1.622243,-2.265597
\H,4.392731,2.254319,-2.885538\H,3.514282,2.186873,-1.344876\C,1.80019
1,2.866849,-3.327674\H,1.578086,3.395528,-2.390743\H,2.520921,3.462296
, -3.91327\H,0.869485,2.794868,-3.914777\C,2.262566,-3.924962,1.75794\H
,3.050176,-4.611691,2.111015\H,2.077261,-3.176,2.541479\H,1.343348,-4.
515226,1.608532\C,4.022086,-2.434825,0.716555\H,3.819994,-1.741941,1.5
48826\H,4.77381,-3.160585,1.075002\C,-3.065571,-3.102405,1.390097\C,-3
.489797,1.756257,-2.18897\C,-4.441039,-3.156591,0.629244\H,-5.113424,-
3.785742,1.239355\C,-4.795134,0.89494,-2.353645\H,-5.582033,1.582249,-
2.711702\H,-4.614582,0.162214,-3.157128\C,-5.262654,0.166339,-1.108012
\C,-6.190435,0.728647,-0.208695\C,-4.750776,-1.113333,-0.82281\C,-6.57
2974,0.029263,0.94582\H,-6.627941,1.709253,-0.421346\C,-5.090272,-1.81
4347,0.349377\H,-4.060268,-1.575178,-1.532233\C,-6.021198,-1.228937,1.
230374\H,-7.309786,0.466033,1.626644\H,-6.328476,-1.766559,2.13311\C,-
2.473988,-4.53498,1.417804\H,-1.519295,-4.558177,1.968894\H,-3.17461,-
5.216871,1.928514\H,-2.296363,-4.912102,0.399647\C,-3.260047,-2.595461
,2.829903\H,-3.922035,-3.288481,3.376398\H,-2.30084,-2.545614,3.367875
\H,-3.717606,-1.596124,2.850261\C,-3.066081,2.267078,-3.590248\H,-3.87

4977,2.881179,-4.020538\H,-2.163162,2.895371,-3.523591\H,-2.858763,1.4
30071,-4.27352\C,-3.737801,2.956912,-1.258794\H,-2.832768,3.575473,-1.
163627\H,-4.537618,3.58795,-1.682025\H,-4.049121,2.638726,-0.253015\H,
-4.276491,-3.686847,-0.322965\H,3.275995,-3.900927,-1.590362\C,2.64165
3,0.749382,-4.412354\H,3.366888,1.337798,-4.999885\H,3.045956,-0.26410
7,-4.276917\H,1.712322,0.669375,-4.995677\C,4.570692,-1.663466,-0.4686
97\C,4.031658,-0.403164,-0.784621\C,5.595099,-2.175946,-1.288355\C,4.4
3401,0.322366,-1.920389\H,3.268716,0.024315,-0.132012\C,6.045875,-1.44
6216,-2.398572\H,6.048165,-3.14409,-1.051445\C,5.462528,-0.211999,-2.7
21351\H,6.853901,-1.844711,-3.019518\H,5.812746,0.343782,-3.597024\C,-
1.310806,3.394768,1.913209\H,-2.133971,3.874251,2.467243\H,-1.594641,3
.269017,0.859511\O,-0.212619,4.311926,2.040931\O,1.855925,5.313278,1.1
08916\S,1.015244,4.132503,0.904358\O,0.391533,3.86223,-0.405415\N,1.93
813,2.839528,1.505298\C,1.409993,1.723575,1.980342\C,0.015929,1.304813
,1.753825\C,2.315201,0.871989,2.79615\C,1.815134,-0.255373,3.484058\C,
3.65761,1.26424,3.001702\C,2.631314,-0.95761,4.379814\H,0.78637,-0.580
643,3.310442\C,4.476173,0.543809,3.875997\H,4.033395,2.147286,2.48111\H
C,3.96375,-0.56265,4.576036\H,2.22777,-1.816868,4.922541\H,5.514124,0.
853813,4.024291\H,4.60124,-1.113034,5.273828\C,-1.050286,1.996093,2.58
81\C,-0.586804,2.241343,4.05096\C,-2.416436,1.277646,2.609269\H,-0.411
692,1.288547,4.573423\H,0.330527,2.844679,4.101727\H,-1.379958,2.78249
3,4.59392\H,-2.818717,1.120987,1.601132\H,-2.324963,0.297982,3.09528\H
, -3.133274,1.883599,3.189509\\Version=ES64L-G16RevA.03\State=1-A\HF=-3
210.8952839\RMSD=6.637e-09\Dipole=-1.4216218,-3.0148393,1.9640503\Quad
rupole=10.4471729,-23.5056407,13.0584679,-21.3937177,-3.2929676,-19.92
49264\PG=C01 [X(C44H53N1O11Rh2S1)]\@

Mf-¹INT6

1\1\GINB-A738\SP\RBPW91\GenECP\C44H53N1O11Rh2S1\SI0C001\05-May-2018\0\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\\Title Card
Required\\0,1\C,0,-0.361726,4.418818,-1.519965\C,0,-1.284362,2.54392,
-2.934143\C,0,-1.527143,3.417619,-1.679268\C,0,-1.676204,2.486645,-0.4
45272\N,0,-2.791376,2.08851,0.102066\S,0,-4.29727,2.670543,-0.436899\O
,0,-3.983662,3.368438,-1.92632\C,0,-2.823951,4.235794,-1.848757\O,0,-5
.174514,1.537238,-0.735524\O,0,-4.696913,3.718251,0.519017\C,0,-0.4379
17,2.018942,0.225986\C,0,0.055372,2.944562,1.248399\C,0,-0.851072,3.59
5465,2.136689\C,0,-0.380214,4.474629,3.115937\C,0,0.989431,4.775535,3.
200242\C,0,1.892724,4.170248,2.309695\C,0,1.439773,3.246673,1.364304\H
,0,-2.810781,4.783492,-2.803693\H,0,-2.957085,4.962672,-1.027854\H,0,-
1.917893,3.374051,2.068393\H,0,-1.089051,4.941928,3.805168\H,0,1.35102
4,5.483487,3.951325\H,0,2.957102,4.417082,2.357677\H,0,2.13824,2.78030
6,0.67087\H,0,-1.107597,3.203191,-3.801952\H,0,-0.40755,1.895418,-2.79
8047\H,0,-2.156282,1.912128,-3.146808\H,0,-0.462016,5.0386,-0.615674\H
,0,0.608188,3.901143,-1.477502\H,0,-0.343706,5.088396,-2.397055\Rh,0,0
.918224,-2.190024,-0.038118\Rh,0,0.234375,0.158725,0.00235\O,0,2.46400

9,-1.767941,1.225682\C,0,2.600861,-0.567684,1.640746\O,0,1.844994,0.42
9823,1.324107\O,0,-0.255679,-2.571862,1.591799\C,0,-0.9348,-1.596517,2
.075986\O,0,-0.928778,-0.390115,1.633673\O,0,-0.637251,-2.573582,-1.30
7753\C,0,-1.422015,-1.621995,-1.658924\O,0,-1.3127,-0.388758,-1.301411
\O,0,2.105794,-1.782503,-1.646583\C,0,2.153681,-0.593079,-2.109356\O,0
,1.488159,0.414511,-1.646736\C,0,3.759847,-0.27854,2.623627\C,0,3.0632
14,-0.329317,-3.330971\C,0,4.557736,-1.565827,2.907986\H,0,5.363501,-1
.344111,3.628516\H,0,3.912753,-2.344494,3.342104\C,0,4.103629,0.795545
, -2.984233\H,0,4.718421,0.945406,-3.889448\H,0,3.546158,1.732225,-2.81
5892\C,0,2.175789,0.175995,-4.496287\H,0,1.646566,1.102107,-4.22645\H,
0,2.803307,0.378621,-5.380354\H,0,1.427383,-0.581524,-4.780878\C,0,3.1
50314,0.2623,3.941563\H,0,3.957495,0.500855,4.654646\H,0,2.556727,1.17
1513,3.765046\H,0,2.498551,-0.492048,4.411915\C,0,4.696902,0.831164,2.
026\H,0,4.119863,1.769415,1.982082\H,0,5.507779,0.98766,2.759414\C,0,-
1.812993,-1.891764,3.312462\C,0,-2.569447,-2.019249,-2.619023\C,0,-2.7
55552,-3.109719,2.998836\H,0,-3.346964,-3.29033,3.914154\C,0,-3.364942
, -3.227773,-2.002733\H,0,-4.155468,-3.481501,-2.731354\H,0,-2.681848,-
4.091303,-1.95056\C,0,-3.97381,-2.982028,-0.635916\C,0,-5.284517,-2.49
3245,-0.47287\C,0,-3.203838,-3.223611,0.516295\C,0,-5.790834,-2.235921
,0.809162\H,0,-5.912784,-2.314823,-1.350812\C,0,-3.676223,-2.927428,1.
807876\H,0,-2.200731,-3.640327,0.402666\C,0,-4.990489,-2.439356,1.9426
43\H,0,-6.812594,-1.863271,0.92428\H,0,-5.39096,-2.222952,2.938202\C,0
, -0.863953,-2.300505,4.468679\H,0,-0.189176,-1.471215,4.737999\H,0,-1.
45836,-2.554812,5.362327\H,0,-0.25247,-3.173759,4.194717\C,0,-2.63111,
-0.652484,3.72096\H,0,-3.242329,-0.894688,4.607022\H,0,-1.971799,0.190
02,3.978974\H,0,-3.30003,-0.321558,2.914069\C,0,-1.915512,-2.503787,-3
.940035\H,0,-2.700365,-2.831544,-4.642341\H,0,-1.351201,-1.689268,-4.4
24126\H,0,-1.22957,-3.345877,-3.762305\C,0,-3.512681,-0.841537,-2.9110
08\H,0,-2.978657,-0.030348,-3.427289\H,0,-4.324333,-1.181208,-3.576726
\H,0,-3.9641,-0.428098,-1.999434\H,0,-2.120378,-3.997332,2.842574\H,0,
5.009922,-1.975536,1.993403\C,0,3.782548,-1.625324,-3.752506\H,0,4.411
347,-1.422443,-4.636122\H,0,4.424414,-2.014318,-2.94928\H,0,3.060292,-
2.412019,-4.017623\C,0,5.283611,0.533932,0.65907\C,0,4.535631,0.824008
, -0.496321\C,0,6.56022,-0.039043,0.49701\C,0,4.995722,0.517643,-1.7894
04\H,0,3.554642,1.291586,-0.38727\C,0,7.05349,-0.322272,-0.785336\H,0,
7.174905,-0.253736,1.376879\C,0,6.275928,-0.054662,-1.921853\H,0,8.052
187,-0.753994,-0.899898\H,0,6.669935,-0.281305,-2.917591\\Version=ES64
L-G09RevD.01\State=1-A\HF=-3210.9083077\RMSD=5.363e-09\Dipole=3.721971
1,1.8303393,-0.389618\Quadrupole=-30.0564377,2.7394772,27.3169605,15.2
906032,3.5368588,-0.8851906\PG=C01 [X(C44H53N1O11Rh2S1)]\@

Bn⁻¹INT1

1\1\GINB-A754\SP\RBPW91\GenECP\C21H27N1O11Rh2S1\SIOC001\17-Mar-2018\0\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\\Title Card

Required\0,1\rh,0,-2.178115,-1.702822,0.715562\rh,0,-1.651703,0.4336
23,-0.289567\o,0,-3.74199,-0.828888,1.692151\c,0,-3.960977,0.421165,1.
50263\o,0,-3.254964,1.202164,0.762978\o,0,-3.411156,-2.145221,-0.84706
2\c,0,-3.535274,-1.265368,-1.774652\o,0,-2.95259,-0.121182,-1.815238\o
,0,-0.61312,-2.550827,-0.273898\c,0,0.089943,-1.794203,-1.037395\o,0,-
0.10474,-0.537361,-1.232712\o,0,-0.930792,-1.231073,2.267123\c,0,-0.34
1212,-0.094343,2.258207\o,0,-0.452335,0.802764,1.338874\n,0,-1.362681,
2.030874,-1.290429\c,0,-5.159948,1.040517,2.183977\c,0,0.560472,0.2486
32,3.421743\c,0,-4.436687,-1.597724,-2.943399\c,0,1.257387,-2.410536,-
1.769733\s,0,0.060212,2.769038,-1.696864\o,0,0.416752,2.260184,-3.0394
07\o,0,-0.160224,4.218419,-1.465097\o,0,1.357388,2.291585,-0.746195\c,
0,1.687242,3.109518,0.407742\h,0,1.421665,4.157515,0.199309\h,0,1.1115
04,2.744762,1.271542\c,0,3.2099,3.01729,0.684031\c,0,4.009399,3.499851
, -0.553588\c,0,3.501271,3.948369,1.894534\c,0,3.610737,1.64053,1.03414
3\c,0,4.007276,0.528098,1.352647\h,0,1.213785,-3.50523,-1.701042\h,0,1
.248358,-2.089355,-2.821718\h,0,2.200112,-2.054673,-1.324424\h,0,0.635
979,-0.604228,4.108516\h,0,1.557251,0.527699,3.045098\h,0,0.150746,1.1
18147,3.960426\h,0,-5.514846,0.391688,2.995452\h,0,-4.904625,2.037879,
2.569782\h,0,-5.968657,1.165516,1.445139\h,0,-5.114342,-0.754984,-3.14
5336\h,0,-3.820399,-1.748198,-3.844431\h,0,-5.011163,-2.509984,-2.7369
8\h,0,4.571966,3.915669,2.147953\h,0,3.233848,4.98996,1.650013\h,0,2.9
30444,3.640179,2.785222\h,0,5.090907,3.464057,-0.349695\h,0,3.793884,2
.86986,-1.428102\h,0,3.733614,4.539582,-0.797511\c,0,4.495638,-0.79936
1,1.734945\h,0,5.313059,-0.680448,2.474022\h,0,3.698137,-1.343682,2.27
6518\c,0,5.001555,-1.687334,0.592647\c,0,5.346878,-3.023734,0.875381\c
,0,5.15268,-1.211225,-0.720329\c,0,5.837093,-3.864764,-0.132206\h,0,5.
231536,-3.408106,1.894776\c,0,5.643332,-2.053617,-1.731846\h,0,4.88307
1,-0.17589,-0.944898\c,0,5.987745,-3.381163,-1.442018\h,0,6.100185,-4.
899831,0.104919\h,0,5.756469,-1.666305,-2.748691\h,0,6.370163,-4.03650
7,-2.229709\Version=ES64L-G09RevD.01\State=1-A\HF=-2318.6372947\RMSD=
3.622e-09\Dipole=-0.4271736,-2.4219609,3.026468\Quadrupole=14.2942837,
-14.1433792,-0.1509045,1.1817645,3.0557849,21.4715694\PG=C01 [X(C21H27
N1O11Rh2S1)]\@

Bn⁻¹TS1

1\1\GINB-A740\SP\RBPW91\GenECP\C21H27N1O11Rh2S1\SIOC001\05-May-2018\0\
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Required\0,1\o,0,-4.165932,0.480961,-0.634224\c,0,-3.459375,1.471251
, -1.045284\o,0,-2.18778,1.587024,-0.918664\o,0,-2.884015,-1.938156,-1.
539764\c,0,-1.816029,-1.663761,-2.195669\o,0,-0.87098,-0.873944,-1.819
378\o,0,-2.194877,-2.560386,1.198287\c,0,-0.924581,-2.479126,1.335258\
o,0,-0.192289,-1.505972,0.915696\o,0,-3.371893,-0.07487,2.084132\c,0,-
2.446158,0.731017,2.461279\o,0,-1.365854,1.01157,1.821537\c,0,-4.17010
9,2.611612,-1.738249\c,0,-2.645803,1.444319,3.783397\c,0,-1.64529,-2.3

01836,-3.556791\C,0,-0.214303,-3.60375,2.054307\H,0,-0.585952,-2.52845
6,-3.740768\H,0,-2.258072,-3.210027,-3.632344\H,0,-1.974239,-1.587051,
-4.329285\H,0,0.190539,-3.230876,3.008995\H,0,-0.911994,-4.427594,2.25
2116\H,0,0.632512,-3.963088,1.450575\H,0,-5.244523,2.40043,-1.815168\H
,0,-4.011293,3.543507,-1.173407\H,0,-3.739136,2.758226,-2.740479\H,0,-
3.449473,0.967301,4.359378\H,0,-1.708702,1.442974,4.35907\H,0,-2.91711
9,2.495335,3.590901\Rh,0,-3.170097,-1.029659,0.280074\C,0,2.223789,3.4
43455,-0.141647\H,0,2.671897,4.422674,-0.377287\H,0,1.149514,3.577011,
0.048027\O,0,2.440194,2.62703,-1.309553\S,0,1.226174,1.525702,-1.71160
8\N,0,0.502097,1.254407,-0.231576\Rh,0,-1.051438,0.106572,-0.025988\C,
0,2.936494,2.836239,1.113633\C,0,4.451767,3.176736,1.055227\C,0,2.2906
99,3.437125,2.385229\O,0,1.978293,0.421384,-2.342539\O,0,0.220629,2.26
9854,-2.513713\C,0,2.811051,1.370327,1.073799\C,0,2.926201,0.150484,0.
9609\H,0,4.892684,2.81374,0.11457\H,0,4.992829,2.71226,1.894197\H,0,1.
23372,3.139834,2.461622\H,0,2.818257,3.093087,3.288793\H,0,4.59093,4.2
70009,1.114399\H,0,2.348636,4.538967,2.355846\C,0,3.129478,-1.282862,0.
.748636\H,0,2.883482,-1.841814,1.668593\H,0,2.411004,-1.616415,-0.0213
57\C,0,4.556311,-1.608077,0.299631\C,0,5.446637,-2.272078,1.160707\C,0
,4.988734,-1.247438,-0.991375\C,0,6.750019,-2.58027,0.740197\H,0,5.118
388,-2.553045,2.167066\C,0,6.290024,-1.555054,-1.410643\H,0,4.300129,-
0.723447,-1.660708\C,0,7.174221,-2.22261,-0.547449\H,0,7.431835,-3.100
066,1.419789\H,0,6.614228,-1.274107,-2.417012\H,0,8.188873,-2.462714,-
0.878283\\Version=ES64L-G09RevD.01\State=1-A\HF=-2318.6297854\RMSD=2.3
46e-09\Dipole=-0.979331,-0.6278825,2.5553657\Quadrupole=-4.7063117,7.4
819568,-2.7756451,-8.3564957,10.5821424,6.4194456\PG=C01 [X(C21H27N1O1
1Rh2S1)]\@

Bn⁻¹INT2

1\1\GINB-A755\SP\RBPW91\GenECP\C21H27N1O11Rh2S1\SIOC001\15-Mar-2018\O\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\\Title Card
Required\\0,1\O,0,-2.448436,2.54662,1.006635\C,0,-1.285961,2.476384,1.
.540227\O,0,-0.417902,1.540578,1.364453\O,0,-2.18083,2.062887,-1.84775
1\C,0,-0.952806,1.833066,-2.129978\O,0,-0.161309,1.027506,-1.510002\O,
0,-3.542001,-0.490209,-1.525074\C,0,-2.704036,-1.444862,-1.692189\O,0,
-1.52707,-1.529741,-1.174846\O,0,-3.808861,0.016102,1.312182\C,0,-3.02
3794,-0.759812,1.968221\O,0,-1.78424,-0.984823,1.711526\C,0,-0.875163,
3.615658,2.454172\C,0,-3.596827,-1.471296,3.177321\C,0,-0.380755,2.558
228,-3.334205\C,0,-3.147784,-2.608244,-2.557554\H,0,-0.918711,3.5013,-
3.502008\H,0,0.693094,2.749143,-3.198683\H,0,-0.50571,1.927901,-4.2307
67\H,0,-3.975765,-2.305574,-3.212467\H,0,-2.306974,-2.989127,-3.154984
\H,0,-3.495048,-3.42799,-1.90668\H,0,-1.752221,4.208673,2.744896\H,0,-
0.369246,3.222966,3.348653\H,0,-0.163362,4.27244,1.926624\H,0,-3.27877
4,-2.524173,3.179707\H,0,-3.203417,-1.004004,4.095163\H,0,-4.692538,-1.
.401191,3.181525\Rh,0,-3.033438,1.056842,-0.27325\C,0,2.090129,-3.2408

28,-1.060652\H,0,2.612594,-4.085462,-1.535484\H,0,1.002853,-3.385388,-
1.173352\O,0,2.458944,-3.287212,0.344872\S,0,1.28614,-2.586052,1.36990
3\N,0,1.054291,-0.953173,0.384481\Rh,0,-0.909655,-0.03877,0.110407\C,0
,2.306029,-0.140195,0.423964\C,0,2.164885,-0.913367,-0.617605\C,0,2.90
9224,0.856601,1.334447\C,0,2.533538,-1.87915,-1.687906\C,0,4.06101,-1.
839209,-1.910322\C,0,1.758342,-1.639331,-3.003597\H,0,4.599164,-2.0952
82,-0.985221\H,0,4.386607,-0.839084,-2.235834\H,0,2.077123,-0.695746,-
3.47123\H,0,0.675404,-1.588842,-2.81981\O,0,2.0144,-2.341285,2.628531\
O,0,0.054304,-3.385288,1.307303\H,0,4.3414,-2.563541,-2.692819\H,0,1.9
65212,-2.461147,-3.709895\C,0,4.234693,1.391139,0.812307\C,0,4.260248,
2.461947,-0.101184\C,0,5.451004,0.812094,1.219551\C,0,5.479238,2.94475
8,-0.598755\H,0,3.318965,2.921171,-0.419458\C,0,6.670955,1.29548,0.724
142\H,0,5.441301,-0.019795,1.930826\C,0,6.687807,2.362054,-0.187238\H,
0,5.485048,3.78055,-1.304311\H,0,7.608968,0.839727,1.053677\H,0,7.6389
11,2.740856,-0.571868\H,0,2.166382,1.660432,1.48197\H,0,3.033807,0.369
25,2.318291\\Version=ES64L-G09RevD.01\State=1-A\HF=-2318.6828465\RMSE=
5.340e-09\Dipole=2.5832315,0.7096736,-2.2332191\Quadrupole=-1.1410845,
-2.7637456,3.9048301,9.5969784,-11.6786845,13.8222947\PG=C01 [X(C21H27
N1O11Rh2S1)]\@

Bn-1TS2

1\1\GINB-A757\SP\BPF91\GenECP\C21H27N1O11Rh2S1\SI0C001\19-Mar-2018\O\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\\Title Card
Required\0,1\C,0,3.381057,2.7739,1.465449\H,0,4.070309,3.186746,2.21
857\H,0,2.575117,3.505989,1.286564\O,0,4.170472,2.594409,0.262954\S,0,
3.222406,2.569664,-1.165414\C,0,2.299062,0.814666,0.668786\Rh,0,-1.073
787,0.017292,-0.00868\N,0,1.815624,1.506272,-0.591226\C,0,2.29732,0.07
3183,-0.402686\C,0,2.789232,1.409427,1.943718\C,0,3.88654,0.510466,2.5
52734\C,0,1.645909,1.669059,2.952449\O,0,4.101232,1.895655,-2.144404\
O,0,2.672892,3.91301,-1.415057\O,0,-3.009488,-2.245315,-0.950315\C,0,-1
.782351,-2.554417,-1.164338\O,0,-0.759196,-1.824695,-0.882296\O,0,-3.2
59517,-1.303179,1.780675\C,0,-2.104537,-1.331884,2.343594\O,0,-1.00958
3,-0.869757,1.850892\O,0,-3.753488,1.38765,0.789817\C,0,-2.738444,2.12
4355,1.072181\O,0,-1.505668,1.824702,0.862335\O,0,-3.501418,0.439326,-
1.918806\C,0,-2.408798,0.902077,-2.418915\O,0,-1.248724,0.858059,-1.86
8489\C,0,-1.511683,-3.913194,-1.775961\C,0,-2.504343,1.587929,-3.76430
3\C,0,-2.033003,-1.939364,3.729504\C,0,-3.01567,3.457373,1.734398\H,0,
-2.815185,-2.70066,3.854456\H,0,-1.040223,-2.375323,3.90764\H,0,-2.201
362,-1.149045,4.480332\H,0,-2.321964,4.220722,1.353879\H,0,-4.055577,3
.763615,1.559537\H,0,-2.854797,3.364912,2.821562\H,0,-1.275985,-4.6326
6,-0.973878\H,0,-2.398424,-4.27326,-2.314454\H,0,-0.647107,-3.865045,-
2.453062\H,0,-3.331841,1.166718,-4.35164\H,0,-2.703356,2.661267,-3.607
206\H,0,-1.554865,1.494487,-4.308867\Rh,0,-3.416979,-0.437507,-0.07325
3\H,0,3.491684,-0.491882,2.781043\H,0,4.731934,0.398017,1.857833\H,0,1

.234852,0.717299,3.320605\H,0,0.824713,2.237795,2.490867\H,0,4.256502,
0.955918,3.491485\H,0,2.032835,2.237686,3.815091\C,0,2.549339,-1.09111
2,-1.283072\H,0,1.590164,-1.613457,-1.452189\H,0,2.865836,-0.684621,-2
.259474\C,0,3.601005,-2.041759,-0.727342\C,0,4.968778,-1.722002,-0.835
892\C,0,3.226442,-3.243464,-0.100076\C,0,5.942564,-2.593078,-0.328625\
H,0,5.2641,-0.786424,-1.320596\C,0,4.20178,-4.114985,0.409269\H,0,2.16
5333,-3.498277,-0.015398\C,0,5.561798,-3.792197,0.295233\H,0,7.001625,
-2.336904,-0.424871\H,0,3.897399,-5.048582,0.891508\H,0,6.322795,-4.47
2726,0.687784\\Version=ES64L-G09RevD.01\State=1-A\HF=-2318.6660645\RMS
D=9.302e-09\Dipole=-0.5083431,-1.9124175,2.6215142\Quadrupole=-14.9366
212,2.6534682,12.2831529,-15.4084926,15.6394225,12.0626611\PG=C01 [X(C
21H27N1O11Rh2S1)]\@

Bn-¹INT3

1\1\GINB-A755\SP\RBPW91\GenECP\C21H27N1O11Rh2S1\SI0C001\15-Mar-2018\0\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\\Title Card
Required\\0,1\C,0,3.084444,2.136654,1.709096\H,0,3.812125,2.084259,2.
533361\H,0,2.660743,3.154026,1.67709\O,0,3.854761,1.898523,0.503\S,0,3
.043588,2.490684,-0.857314\C,0,1.359303,0.830258,0.561695\Rh,0,-0.7068
11,0.040167,-0.029976\C,0,1.529398,0.20686,-0.628082\N,0,1.425516,1.70
9293,-0.693131\C,0,2.173294,-0.799366,-1.532225\C,0,1.962086,1.073198,
1.929936\C,0,2.564654,-0.241626,2.471386\C,0,0.976922,1.687035,2.95049
5\O,0,3.801715,1.953546,-2.001412\O,0,2.808862,3.935103,-0.709539\O,0,
-2.732387,-2.272045,-0.877435\C,0,-1.512895,-2.629601,-1.011611\O,0,-0
.476367,-1.91218,-0.737909\O,0,-3.002612,-1.207134,1.784031\C,0,-1.861
985,-1.236377,2.361637\O,0,-0.75287,-0.781985,1.886225\O,0,-3.48775,1.
435147,0.653398\C,0,-2.490497,2.217733,0.837437\O,0,-1.251339,1.92947,
0.6477\O,0,-3.190201,0.364804,-1.983935\C,0,-2.09328,0.757984,-2.51927
9\O,0,-0.926173,0.72255,-1.97945\C,0,-1.248111,-4.031439,-1.522548\C,0
, -2.160127,1.326758,-3.921287\C,0,-1.792952,-1.863765,3.740049\C,0,-2.
780921,3.617905,1.337809\H,0,-1.10757,-2.725949,3.723215\H,0,-1.391397
, -1.138332,4.46483\H,0,-2.790196,-2.192183,4.059923\H,0,-3.858739,3.82
2023,1.296219\H,0,-2.433301,3.718444,2.378888\H,0,-2.230641,4.353142,0
.731838\H,0,-2.17522,-4.476805,-1.906076\H,0,-0.481664,-4.013772,-2.31
1558\H,0,-0.864236,-4.656237,-0.699404\H,0,-1.806133,2.369557,-3.91213
9\H,0,-1.490268,0.759428,-4.586049\H,0,-3.188206,1.285143,-4.30364\Rh,
0,-3.106625,-0.420284,-0.103093\H,0,1.791382,-1.019341,2.544763\H,0,3.
371538,-0.607764,1.820331\H,0,2.977962,-0.066552,3.479774\H,0,0.204861
,0.956367,3.222448\H,0,1.528565,1.972218,3.862884\H,0,0.483898,2.58046
6,2.541277\C,0,3.203215,-1.705117,-0.865424\C,0,4.567428,-1.354161,-0.
873199\C,0,2.812923,-2.911137,-0.252522\C,0,5.520185,-2.193533,-0.2765
2\H,0,4.879095,-0.419706,-1.346945\C,0,3.765816,-3.748967,0.34503\H,0,
1.754648,-3.184902,-0.244499\C,0,5.123045,-3.39231,0.335373\H,0,6.5765
02,-1.909642,-0.293719\H,0,3.44804,-4.684714,0.814988\H,0,5.867396,-4.

046896,0.798019\H,0,1.372238,-1.407689,-1.982042\H,0,2.64036,-0.223649
, -2.347595\\Version=ES64L-G09RevD.01\State=1-A\HF=-2318.6668292\RMSD=6
.884e-09\Dipole=-0.8888634,-1.9880152,2.1232802\Quadrupole=-17.5989576
,2.2205172,15.3784404,-14.2197344,12.4371281,7.5409582\PG=C01 [X(C21H2
7N1O11Rh2S1)]\@

Bn-¹TS3

1\1\GINB-A759\SP\RBPW91\GenECP\C21H25N1O11Rh2S1\SIOC001\14-Mar-2018\0\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\Title Card
Required\0,1\C,0,-3.391489,-2.131143,1.689\H,0,-4.128602,-2.132082,2
.504673\H,0,-2.751867,-3.026042,1.783593\O,0,-4.175666,-2.207886,0.464
71\S,0,-3.238358,-2.585405,-0.894965\C,0,-1.844231,-0.772273,0.417811\
Rh,0,0.723077,-0.069689,-0.122639\C,0,-1.3507,-0.092772,-0.666312\N,0,
-1.690269,-1.794344,-0.525788\C,0,-1.999178,0.817453,-1.686255\C,0,-2.
573101,-0.845924,1.67539\C,0,-3.106216,0.42591,2.344223\C,0,-1.978826,
-0.311965,2.989826\O,0,-3.940666,-1.945026,-2.020412\O,0,-2.946433,-4.
024413,-0.89673\O,0,3.141218,1.718233,-1.216679\C,0,2.024385,2.022576,
-1.760648\O,0,0.879433,1.490861,-1.499686\O,0,2.71496,1.611889,1.64187
3\C,0,1.496133,1.855301,1.941142\O,0,0.452234,1.320201,1.402583\O,0,3.
107019,-1.283696,1.556168\C,0,2.002678,-1.890437,1.783379\O,0,0.857116
, -1.608379,1.266871\O,0,3.450149,-1.157547,-1.292179\C,0,2.425276,-1.6
72174,-1.868631\O,0,1.191381,-1.418738,-1.608214\C,0,2.040515,3.092159
, -2.8348\C,0,2.676949,-2.670295,-2.980781\C,0,1.250718,2.848297,3.0613
39\C,0,2.034909,-3.066826,2.738386\H,0,2.027877,3.625281,3.051728\H,0,
0.254144,3.301191,2.972\H,0,1.31147,2.324998,4.03055\H,0,3.020863,-3.1
47422,3.214142\H,0,1.253758,-2.956416,3.505873\H,0,1.82105,-3.993345,2
.181329\H,0,2.988988,3.644463,-2.809328\H,0,1.931567,2.615779,-3.82324
1\H,0,1.194243,3.782488,-2.704371\H,0,2.415788,-2.212391,-3.948886\H,0
,3.732989,-2.96979,-2.996926\H,0,2.030733,-3.550582,-2.847795\Rh,0,3.1
30449,0.228293,0.179448\H,0,-2.178277,-0.926636,3.872865\H,0,-0.975783
,0.109642,2.922184\H,0,-4.108394,0.34889,2.774582\H,0,-2.889405,1.3716
02,1.844487\C,0,-2.828739,1.932188,-1.064809\C,0,-4.228004,1.808683,-0
.955086\C,0,-2.209656,3.105683,-0.589636\C,0,-4.991705,2.836546,-0.381
703\H,0,-4.718219,0.903164,-1.324817\C,0,-2.973174,4.131672,-0.012932\
H,0,-1.124554,3.206535,-0.67462\C,0,-4.366765,3.999958,0.093579\H,0,-6
.078153,2.729355,-0.311546\H,0,-2.479181,5.038991,0.34782\H,0,-4.96251
3,4.802456,0.538107\H,0,-2.643608,0.171228,-2.305905\H,0,-1.212627,1.2
28654,-2.33429\\Version=ES64L-G09RevD.01\State=1-A\HF=-2317.4282102\RM
SD=4.745e-09\Dipole=-0.1729363,1.9441572,2.62119\Quadrupole=-15.618234
4,-0.6466602,16.2648946,-13.5506657,-20.7332925,-9.0905366\PG=C01 [X(C
21H25N1O11Rh2S1)]\@

Bn-¹INT4

1\1\GINB-A751\SP\RBPW91\GenECP\C21H27N1O11Rh2S1\SIOC001\11-Mar-2018\0\
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\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\Title Card
Required\0,1\rh,0,0.856571,-0.141108,-0.053733\rh,0,3.282112,0.21835
,-0.023478\o,0,1.27032,-2.175977,-0.159902\c,0,2.502612,-2.563358,-0.1
87388\o,0,3.53568,-1.811708,-0.154342\o,0,0.97924,-0.258437,2.015827\c
,0,2.127016,-0.128341,2.596066\o,0,3.246823,0.073857,2.016486\o,0,0.66
5402,1.913474,0.046771\c,0,1.725932,2.647758,0.097509\o,0,2.937467,2.2
34759,0.098824\o,0,1.018817,-0.025421,-2.117121\c,0,2.162642,0.201079,
-2.668908\o,0,3.27748,0.357023,-2.062497\c,0,2.727193,-4.06121,-0.2479
28\c,0,2.161851,0.276937,-4.181255\c,0,2.121797,-0.222447,4.108263\c,0
,1.490879,4.141485,0.186382\c,0,-2.546223,-0.621815,2.328022\c,0,-1.66
907,1.755712,2.29989\c,0,-2.571828,0.725347,1.57455\c,0,-2.117815,0.54
7819,0.112112\n,0,-2.588876,1.197758,-0.92086\s,0,-3.797073,2.388614,-
0.77295\o,0,-4.080343,2.537421,0.867784\c,0,-4.021512,1.250227,1.53995
6\o,0,-3.252889,3.685242,-1.183089\o,0,-4.987697,1.812828,-1.421165\c,
0,-1.066077,-0.422448,-0.286893\h,0,-4.388101,1.447228,2.558631\h,0,-4
.706019,0.535039,1.050163\h,0,0.634761,4.430378,-0.43969\h,0,1.251847,
4.411383,1.228556\h,0,2.394167,4.686268,-0.118663\h,0,3.153192,0.57350
3,-4.547324\h,0,1.895021,-0.706491,-4.600652\h,0,1.401789,0.9975,-4.51
952\h,0,1.526852,0.603286,4.530291\h,0,1.649662,-1.165062,4.425511\h,0
,3.147378,-0.169082,4.495348\h,0,2.41164,-4.518737,0.703925\h,0,2.1153
54,-4.505238,-1.047629\h,0,3.788925,-4.280272,-0.419576\h,0,-2.058648,
1.905158,3.322312\h,0,-0.639171,1.384793,2.367353\h,0,-1.668329,2.7245
69,1.782545\h,0,-3.207226,-1.369862,1.864949\h,0,-1.523507,-1.027926,2
.358191\h,0,-2.876656,-0.46438,3.36907\c,0,-1.510408,-1.49452,-1.25093
7\h,0,-0.655681,-2.129342,-1.522794\h,0,-1.814417,-0.933335,-2.159531\
c,0,-2.67809,-2.352819,-0.769883\c,0,-4.015238,-2.01125,-1.054202\c,0,
-2.414342,-3.520248,-0.025997\c,0,-5.066236,-2.823512,-0.600393\h,0,-4
.235889,-1.110275,-1.633398\c,0,-3.465696,-4.331238,0.425649\h,0,-1.37
7033,-3.791333,0.1923\c,0,-4.79542,-3.983923,0.141315\h,0,-6.098742,-2
.551164,-0.837348\h,0,-3.245002,-5.23703,0.99821\h,0,-5.615778,-4.6174
99,0.490304\Version=ES64L-G09RevD.01\State=1-A\HF=-2318.6946075\RMSD=
5.751e-09\Dipole=0.8850657,-2.6731718,2.257262\Quadrupole=-20.0718836,
2.4958441,17.5760395,14.2507862,-16.0492074,5.4037609\PG=C01 [X(C21H27
N1O11Rh2S1)]\@

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Bn-1TS4-1

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1\1\GINB-A751\SP\RBPW91\GenECP\C21H27N1O11Rh2S1\SIOC001\11-Mar-2018\0\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\Title Card
Required\0,1\rh,0,-0.84269666,0.28089887,0.\o,0,1.67645634,0.9924808
7,-1.687243\c,0,0.60497234,0.96577187,-2.407499\o,0,-0.57435466,0.7052
5987,-1.989849\o,0,1.18815634,2.54693187,0.716815\c,0,-0.02893266,2.97
688487,0.668887\o,0,-1.06934866,2.28309887,0.404593\o,0,1.20733234,0.1
2200287,2.334894\c,0,0.00206834,-0.12140613,2.725834\o,0,-1.04602566,-
0.13697213,1.992363\o,0,1.74302134,-1.47071213,-0.083987\c,0,0.6825683

```

4,-2.14795313,-0.362969\O,0,-0.51833666,-1.70034513,-0.401825\C,0,0.78
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0.22675566,4.45361887,0.95384\C,0,-0.17394766,-0.41963713,4.202148\C,0
,5.11435134,0.39067087,2.942048\C,0,3.90930034,-1.78493013,2.463015\C,
0,4.97503534,-0.78310113,1.948255\C,0,4.58093134,-0.28503213,0.541516\
N,0,4.95125834,-0.81239213,-0.596499\S,0,6.06436034,-2.08961113,-0.667
609\O,0,6.24323534,-2.61931013,0.910399\C,0,6.33373534,-1.50409613,1.8
34561\O,0,5.46808234,-3.22114713,-1.379785\O,0,7.33258734,-1.48256413,
-1.113885\H,0,6.61272034,-1.95592213,2.798629\H,0,7.14250634,-0.819754
13,1.520765\H,0,0.20978534,4.70892987,1.932121\H,0,0.29584434,5.053431
87,0.19128\H,0,-1.29501466,4.70531587,0.946325\H,0,0.23601934,0.407180
87,4.802985\H,0,-1.23601666,-0.56149613,4.439938\H,0,0.38696734,-1.329
97313,4.467828\H,0,1.35986834,0.43978587,-4.348919\H,0,-0.19091166,1.3
4358987,-4.377567\H,0,1.36183634,2.18427287,-4.019386\H,0,0.77571034,-
4.18957613,0.29622\H,0,0.12147234,-3.98246313,-1.347483\H,0,1.89330234
, -3.80370913,-1.041155\C,0,4.12804334,2.19249487,0.241265\H,0,3.671488
34,1.33363287,-0.750942\C,0,3.64962934,0.86254187,0.42969\Rh,0,1.55887
834,0.53901087,0.3298\C,0,5.47376634,2.78494087,0.156817\C,0,6.6708593
4,2.07699687,-0.116716\C,0,5.54615534,4.18668787,0.359815\C,0,7.893856
34,2.75514487,-0.157909\H,0,6.64875134,1.01233787,-0.349204\C,0,6.7751
1434,4.85313287,0.342001\H,0,4.62544034,4.74680487,0.550204\C,0,7.9546
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34934,2.92988287,0.195642\H,0,5.87084234,1.12304087,2.61812\H,0,4.1529
4234,0.91101587,3.070933\H,0,5.41718634,0.00114587,3.928641\H,0,4.2198
2334,-2.14921113,3.458221\H,0,2.92960734,-1.29848013,2.553452\H,0,3.81
664134,-2.64722713,1.789028\\Version=ES64L-G09RevD.01\State=1-A\HF=-23
18.6729608\RMSD=1.898e-09\Dipole=0.9725952,3.5684262,2.5414845\Quadrup
ole=-15.507501,7.9079165,7.5995845,20.9666615,13.4030906,-10.8958265\P
G=C01 [X(C21H27N1O11Rh2S1)]\@

Bn⁻¹TS4-2

1\1\GINB-A745\SP\RBPW91\GenECP\C21H27N1O11Rh2S1\SIOC001\05-May-2018\0\
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, -1.844498\C,0,-1.604991,0.670179,-2.658988\O,0,-2.82083,0.393473,-2.3
63676\O,0,-1.319649,2.215189,0.540713\C,0,-2.52987,2.636872,0.37442\O,
0,-3.529624,1.938943,-0.006647\O,0,-1.398646,-0.237006,2.104896\C,0,-2
.634621,-0.489489,2.380964\O,0,-3.609474,-0.500658,1.5535\O,0,-0.65860
4,-1.785786,-0.273002\C,0,-1.681394,-2.4676,-0.661429\O,0,-2.876964,-2
.028578,-0.809263\C,0,-1.288136,0.96851,-4.110378\C,0,-1.435187,-3.935
557,-0.942877\C,0,-2.76775,4.108651,0.653495\C,0,-2.949282,-0.779884,3
.83572\C,0,2.900416,-0.118374,2.790851\C,0,1.37882,-2.09896,2.363559\C
,0,2.515147,-1.22239,1.779941\C,0,2.072046,-0.626208,0.42357\N,0,2.353

01,-1.106584,-0.758066\S,0,3.313263,-2.48175,-0.967783\O,0,3.485276,-3.133464,0.565402\C,0,3.76542,-2.095063,1.536661\O,0,2.567628,-3.491217,-1.721917\O,0,4.62279,-1.99061,-1.434323\H,0,4.044098,-2.631137,2.456597\H,0,4.630706,-1.493308,1.204617\H,0,-2.36781,4.375541,1.643897\H,0,-2.235007,4.717725,-0.094999\H,0,-3.840167,4.338071,0.608602\H,0,-2.233463,-1.510335,4.241857\H,0,-2.848963,0.146193,4.425509\H,0,-3.974134,-1.159967,3.936399\H,0,-0.759533,0.106315,-4.54906\H,0,-2.212162,1.149208,-4.675136\H,0,-0.618636,1.838298,-4.183235\H,0,-1.550679,-4.509025,-0.007525\H,0,-2.170969,-4.310416,-1.667465\H,0,-0.412197,-4.08601,-1.314289\C,0,1.643358,1.87883,0.204711\H,0,1.328033,1.373426,1.373561\C,0,1.155149,0.540844,0.358997\Rh,0,-0.887651,0.219396,0.144934\C,0,2.998838,2.437416,0.001878\C,0,4.091511,1.721407,-0.543965\C,0,3.181316,3.800429,0.34456\C,0,5.327807,2.355645,-0.719935\H,0,3.968027,0.68997,-0.872599\C,0,4.421467,4.423655,0.177771\H,0,2.33692,4.366748,0.750375\C,0,5.50124,3.699775,-0.35387\H,0,6.156869,1.79424,-1.158785\H,0,4.544953,5.474232,0.454422\H,0,6.470701,4.185816,-0.494321\H,0,0.837258,2.625783,0.169178\H,0,3.632629,0.594703,2.378112\H,0,2.014973,0.438121,3.140526\H,0,3.349766,-0.582105,3.685465\H,0,1.707153,-2.507526,3.335607\H,0,0.462871,-1.51159,2.515013\H,0,1.145904,-2.935333,1.690925\\Version=ES64L-G09RevD.01\State=1-A\HF=-2318.6729199\RMSD=5.521e-09\Dipole=1.3131546,3.3734681,3.4982011\Quadrupole=-13.2367835,6.2307568,7.0060267,17.5880312,12.014518,-8.8626492\PG=C01 [X(C21H27N1O11Rh2S1)]\@

Bn-1TS5-1

1\1\GINB-A751\SP\RBPW91\GenECP\C21H27N1O11Rh2S1\SIOC001\12-Mar-2018\O\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\\Title Card Required\\0,1\Rh,0,2.898368,-0.548138,0.719377\O,0,0.587065,1.455289,1.274374\C,0,1.561118,1.594589,2.107215\O,0,2.6651,0.946223,2.096282\O,0,1.748065,1.395415,-1.456472\C,0,3.038555,1.432509,-1.393642\O,0,3.779897,0.756011,-0.604872\O,0,1.104692,-1.391203,-1.679391\C,0,2.167621,-2.117234,-1.584635\O,0,3.066983,-2.033138,-0.679741\O,0,-0.093082,-1.325796,1.072261\C,0,0.669393,-1.933404,1.91426\O,0,1.942346,-1.815882,2.011015\C,0,1.351845,2.602563,3.218362\C,0,-0.016794,-2.89617,2.861579\C,0,3.739601,2.351848,-2.376964\C,0,2.341455,-3.189779,-2.641129\C,0,-2.508947,-1.339943,-3.035289\C,0,-1.79912,-2.794542,-1.108231\C,0,-2.648454,-1.564618,-1.515127\C,0,-2.258608,-0.318563,-0.659722\N,0,-2.827451,-0.018389,0.479848\S,0,-4.128681,-0.858192,1.132444\O,0,-4.34743,-2.20828,0.160455\C,0,-4.136496,-1.879183,-1.231514\O,0,-3.76095,-1.398449,2.444925\O,0,-5.297227,0.026718,0.975141\H,0,-4.44336,-2.779627,-1.785832\H,0,-4.799615,-1.044607,-1.526956\H,0,4.58318,2.857608,-1.885419\H,0,4.148743,1.750253,-3.20572\H,0,3.041817,3.091075,-2.792765\H,0,2.022541,-2.807259,-3.621819\H,0,3.383691,-3.531993,-2.682182\H,0,1.695741,-4.050006,-2.394334\H,0,2.311297,2.861746,3.684913\H,0,0.849987,3.502323,2.835084\H,0,0.693201,2.15837,3.983553\H,0,0.53016,-2.94222

7, 3.813702\H, 0, -1.059649, -2.593474, 3.026832\H, 0, -0.011709, -3.906508, 2.418419\C, 0, -1.135224, 0.568059, -1.082457\Rh, 0, 0.718464, 0.05334, -0.227136\H, 0, -0.272564, 1.695528, -2.737251\H, 0, -2.060938, 1.3322, -2.971551\C, 0, -1.567553, 2.297032, -1.026948\C, 0, -1.217018, 1.389119, -2.275815\C, 0, -2.948693, 2.607892, -0.815617\C, 0, -0.597756, 3.264008, -0.611089\C, 0, -3.332446, 3.809655, -0.227102\H, 0, -3.715512, 1.884796, -1.094914\C, 0, -0.994131, 4.472905, -0.045872\H, 0, 0.456284, 3.040529, -0.773144\C, 0, -2.358788, 4.750368, 0.151364\H, 0, -4.392784, 4.01958, -0.06785\H, 0, -0.23884, 5.207561, 0.245941\H, 0, -2.664093, 5.701092, 0.597372\H, 0, -2.818018, -2.259763, -3.560646\H, 0, -3.149683, -0.521821, -3.404434\H, 0, -1.466683, -1.132056, -3.316814\H, 0, -0.73778, -2.613899, -1.318185\H, 0, -1.91559, -3.024477, -0.041708\H, 0, -2.137249, -3.667176, -1.694765\Version=ES64L-G09RevD.01\State=1-A\HF=-2318.6673849\RMSD=1.846e-09\Dipole=0.2775763, 1.9990169, -3.9527808\Quadrupole=-29.0957302, 23.7358493, 5.3598809, -1.7930586, 14.775506, 9.0642982\PG=C01 [X(C21H27N1O11Rh2S1)]\@

Bn⁻¹TS5-2

1\1\GINB-A755\SP\RBPW91\GenECP\C21H27N1O11Rh2S1\SI0C001\15-Mar-2018\0\
\#p genecp scrf=(iefpcm, solvent=dichloromethane, smd) bpw91\Title Card
Required\0, 1\Rh, 0, -0.805518, 0.13789, -0.094228\Rh, 0, -3.072839, -0.767353, 0.131406\O, 0, -1.693768, 2.011523, -0.0746\C, 0, -2.957751, 2.117359, 0.16811\O, 0, -3.772265, 1.149305, 0.338876\O, 0, -0.766427, 0.236601, 1.976177\C, 0, -1.738686, -0.283938, 2.646806\O, 0, -2.777427, -0.852277, 2.161743\O, 0, -0.181918, -1.843396, -0.129458\C, 0, -1.055774, -2.786827, -0.185161\O, 0, -2.327607, -2.651593, -0.091755\O, 0, -1.112358, 0.010495, -2.147029\C, 0, -2.276131, -0.311056, -2.597544\O, 0, -3.297064, -0.643825, -1.899693\C, 0, -3.514878, 3.525639, 0.242477\C, 0, -2.455081, -0.236773, -4.101702\C, 0, -1.64769, -0.193514, 4.157627\C, 0, -0.527935, -4.183653, -0.437522\C, 0, 2.413353, 0.97274, 2.27152\C, 0, 1.984527, -1.511254, 2.111097\C, 0, 2.723665, -0.305708, 1.467217\C, 0, 2.353437, -0.19897, -0.030149\N, 0, 2.962369, -0.873062, -0.970697\S, 0, 4.330053, -1.837903, -0.700718\O, 0, 4.587337, -1.849645, 0.953238\C, 0, 4.242583, -0.579381, 1.560702\O, 0, 4.038041, -3.230568, -1.0489\O, 0, 5.431876, -1.096492, -1.340658\C, 0, 1.235474, 0.682574, -0.551009\H, 0, 4.545858, -0.684559, 2.613399\H, 0, 4.842238, 0.230483, 1.105284\H, 0, -1.267721, -4.936279, -0.134106\H, 0, -0.346983, -4.295939, -1.520714\H, 0, 0.433761, -4.339509, 0.068688\H, 0, -1.48734, -0.330278, -4.612316\H, 0, -3.158246, -1.00742, -4.44517\H, 0, -2.879148, 0.749527, -4.361472\H, 0, -1.903964, -1.163922, 4.606498\H, 0, -0.642497, 0.115785, 4.474313\H, 0, -2.377155, 0.549326, 4.52032\H, 0, -2.942368, 4.122496, 0.969345\H, 0, -3.418386, 4.015089, -0.740405\H, 0, -4.573573, 3.502064, 0.53112\H, 0, 2.289502, -1.583214, 3.169869\H, 0, 0.900533, -1.370463, 2.063595\H, 0, 2.245343, -2.454453, 1.612585\H, 0, 2.992621, 1.84066, 1.920512\H, 0, 1.343176, 1.213953, 2.218609\H, 0, 2.672161, 0.801001, 3.330323\C, 0, 1.836929, 2.285384, -0.718545\C, 0, 1.461473, 1.228004, -1.870066\H, 0, 0.599614, 1.573301, -2.444158\H, 0, 2.334677, 0.934051, -2.464647\C, 0, 3.250353, 2.505511

, -0.584538\C, 0, 0.969083, 3.40681, -0.504577\C, 0, 3.756861, 3.760066, -0.248
122\H, 0, 3.936697, 1.676131, -0.77172\C, 0, 1.487885, 4.651795, -0.164848\H, 0
, -0.108847, 3.250335, -0.574312\C, 0, 2.879423, 4.837196, -0.038668\H, 0, 4.83
683, 3.905806, -0.163405\H, 0, 0.810272, 5.493274, 0.003141\H, 0, 3.277479, 5.8
23386, 0.216055\\Version=ES64L-G09RevD.01\State=1-A\HF=-2318.6597706\RM
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78, 16.0885193, 10.9304685, 19.9276231, 16.9817435, -4.1825083\PG=C01 [X(C2
1H27N1O11Rh2S1)]\@

Bn⁻¹PC1

1\1\GINB-A723\SP\RBPW91\GenECP\C21H27N1O11Rh2S1\SIOC001\26-Apr-2018\0\
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Required\0, 1\Rh, 0, 1.361853, 0.124348, -0.052202\Rh, 0, 3.699404, 0.483361
, 0.346956\O, 0, 1.408383, -1.362898, 1.38452\C, 0, 2.528621, -1.607707, 1.9665
47\O, 0, 3.644095, -1.009147, 1.755116\O, 0, 0.959907, 1.519367, 1.412323\C, 0,
1.950758, 2.085172, 2.001239\O, 0, 3.197169, 1.862313, 1.780505\O, 0, 1.435053
, 1.625333, -1.454788\C, 0, 2.557232, 2.214485, -1.662039\O, 0, 3.673071, 1.955
836, -1.078017\O, 0, 1.88646, -1.25406, -1.489038\C, 0, 3.13419, -1.461718, -1.
713156\O, 0, 4.119568, -0.905685, -1.103737\C, 0, 2.531234, -2.726165, 2.99185
9\C, 0, 3.475272, -2.432946, -2.825685\C, 0, 1.619893, 3.141985, 3.037177\C, 0,
2.557027, 3.345303, -2.671416\C, 0, -3.669823, -3.266792, 1.902413\C, 0, -3.99
3029, -4.06023, -0.499157\C, 0, -3.38464, -2.961092, 0.411131\C, 0, -3.977723,
-1.589044, -0.007958\N, 0, -3.349556, -0.687823, -0.726539\S, 0, -1.77114, -0.
905687, -1.270092\O, 0, -1.456911, -2.521921, -1.074415\C, 0, -1.84973, -2.952
295, 0.259394\O, 0, -1.71918, -0.667244, -2.710038\O, 0, -0.940589, -0.109438,
-0.323758\C, 0, -5.357795, -1.343724, 0.39801\H, 0, -1.445829, -3.970827, 0.35
306\H, 0, -1.358645, -2.311846, 1.010909\H, 0, 2.381837, 3.151446, 3.829231\H,
0, 1.61822, 4.133866, 2.554763\H, 0, 0.623181, 2.963877, 3.463444\H, 0, 1.80468
3, 3.161301, -3.450941\H, 0, 2.296968, 4.287295, -2.159839\H, 0, 3.554466, 3.46
0489, -3.117532\H, 0, 1.69149, -2.598822, 3.691955\H, 0, 2.395765, -3.693572, 2
.480811\H, 0, 3.480512, -2.741613, 3.543015\H, 0, 4.436465, -2.925574, -2.6231
13\H, 0, 2.676014, -3.177456, -2.943987\H, 0, 3.567804, -1.876282, -3.773374\H
, 0, -3.633597, -5.051025, -0.173168\H, 0, -5.093132, -4.068112, -0.449881\H, 0
, -3.695553, -3.912712, -1.548285\H, 0, -3.351113, -2.438112, 2.55474\H, 0, -4.
734289, -3.466212, 2.09453\H, 0, -3.11172, -4.170712, 2.201958\C, 0, -6.167347
, -0.232316, 0.459354\H, 0, -7.165591, -0.483327, 0.842446\C, 0, -6.050388, 1.2
022, 0.216095\C, 0, -7.17335, 1.986531, 0.604623\C, 0, -4.936453, 1.875814, -0.
349797\C, 0, -7.181278, 3.37411, 0.452472\H, 0, -8.044929, 1.48734, 1.040475\C
, 0, -4.948303, 3.266171, -0.497523\H, 0, -4.078315, 1.292566, -0.679288\C, 0, -
6.063139, 4.021301, -0.098969\H, 0, -8.056398, 3.951893, 0.762145\H, 0, -4.078
493, 3.763191, -0.935642\H, 0, -6.064092, 5.108022, -0.222664\H, 0, -5.850698,
-2.25012, 0.760496\\Version=ES64L-G09RevD.01\State=1-A\HF=-2318.7414132
\RMSD=3.158e-09\Dipole=-3.5009728, -1.5434314, 2.0547899\Quadrupole=6.60
53632, 13.1869243, -19.7922875, 4.1053562, -16.9735466, -7.3858689\PG=C01 [

X(C21H27N1O11Rh2S1)]\@

Bn-1P1

1\1\GINB-A750\SP\RBPW91\6-311++G(d,p)\C13H15N1O3S1\SIOC001\11-Apr-2018
\0\#p scrf=(iefpcm,solvent=dichloromethane,smd) bpw91/6-311++G(d,p)\
Title Card Required\0,1\C,0,-2.544454,2.500127,0.95922\C,0,-2.461637,
1.865053,-1.505984\C,0,-2.266856,1.360429,-0.053081\C,0,-0.821898,0.80
8161,0.081303\N,0,-0.510218,-0.462248,0.157551\S,0,-1.655294,-1.699402
,0.071149\O,0,-3.030637,-0.946904,-0.515721\C,0,-3.295231,0.251943,0.2
54899\O,0,-1.242526,-2.611725,-0.997301\O,0,-1.904774,-2.183038,1.4396
36\C,0,0.241647,1.809055,0.093104\H,0,-4.304962,0.570516,-0.045239\H,0
, -3.312113,0.003698,1.330986\H,0,-3.45702,2.329715,-1.609245\H,0,-1.70
4996,2.618581,-1.775457\H,0,-2.391821,1.033083,-2.222909\H,0,-2.257606
,2.216033,1.984347\H,0,-2.021638,3.432324,0.699116\H,0,-3.624161,2.729
452,0.960022\C,0,1.617366,1.764506,0.090043\H,0,2.048999,2.774194,0.11
6968\C,0,2.672439,0.756151,0.044457\C,0,4.003723,1.25944,0.079641\C,0,
2.499503,-0.649356,-0.05172\C,0,5.10805,0.408025,0.025601\H,0,4.160709
,2.340818,0.149538\C,0,3.609523,-1.497145,-0.114161\H,0,1.489786,-1.05
6493,-0.072916\C,0,4.913674,-0.97924,-0.073144\H,0,6.119215,0.822963,0
.057299\H,0,3.452106,-2.576452,-0.191316\H,0,5.774718,-1.652313,-0.117
313\H,0,-0.146566,2.830495,0.100902\Version=ES64L-G09RevD.01\State=1-
A\HF=-1183.1050988\RMSD=5.223e-09\Dipole=0.5338812,3.6766155,0.0927162
\Quadrupole=14.5535829,-3.5770357,-10.9765472,-11.1164479,-0.7284502,0
.4879104\PG=C01 [X(C13H15N1O3S1)]\@

Bn-1PC2

1\1\GINB-A749\SP\RBPW91\GenECP\C21H27N1O11Rh2S1\SIOC001\03-May-2018\0\
\#p genecp scrf=(iefpcm,solvent=dichloromethane,smd) bpw91\Title Card
Required\0,1\Rh,0,-0.747213,-0.128211,0.084694\Rh,0,-2.950031,0.8533
93,-0.049033\O,0,-0.039449,1.531015,-0.919539\C,0,-0.869979,2.454544,-
1.25267\O,0,-2.129583,2.468204,-1.008756\O,0,-0.565731,0.835684,1.9219
14\C,0,-1.536519,1.560949,2.349225\O,0,-2.655165,1.763085,1.755358\O,0
, -1.624909,-1.686657,1.118727\C,0,-2.896369,-1.689519,1.292911\O,0,-3.
721501,-0.78365,0.904168\O,0,-1.133909,-1.003033,-1.731316\C,0,-2.2705
8,-0.811389,-2.29885\O,0,-3.223184,-0.075383,-1.853297\C,0,-0.312396,3
.625468,-2.037453\C,0,-2.510291,-1.550441,-3.598573\C,0,-1.328783,2.27
0011,3.674503\C,0,-3.471771,-2.88518,2.025547\C,0,5.066896,-0.959708,0
.514585\C,0,3.701242,-2.289064,2.175968\C,0,3.743634,-1.728746,0.72398
9\C,0,2.487578,-0.830823,0.571595\N,0,1.321358,-1.185774,0.086124\S,0,
1.227016,-2.723743,-0.81371\O,0,2.475713,-3.61882,-0.173349\C,0,3.7307
61,-2.898891,-0.269194\O,0,0.032544,-3.465969,-0.431446\O,0,1.553921,-
2.372681,-2.204109\C,0,2.606643,0.562616,1.127784\H,0,4.505003,-3.6377
37,-0.013059\H,0,3.888747,-2.563515,-1.308226\H,0,-2.291682,2.598363,4
.087786\H,0,-0.815713,1.6083,4.387439\H,0,-0.692336,3.156851,3.517574\

H, 0, -3.246619, -3.803829, 1.461409\H, 0, -2.994205, -2.981318, 3.013255\H, 0, -4.557677, -2.778664, 2.146175\H, 0, 0.742771, 3.793909, -1.783862\H, 0, -0.376148, 3.398459, -3.115112\H, 0, -0.906759, 4.529318, -1.844444\H, 0, -3.230334, -1.003674, -4.222892\H, 0, -1.562819, -1.697981, -4.134655\H, 0, -2.931697, -2.544237, -3.372205\H, 0, 4.596306, -2.911267, 2.345793\H, 0, 3.709838, -1.472862, 2.913157\H, 0, 2.809176, -2.911337, 2.340339\H, 0, 5.134946, -0.516525, -0.49018\H, 0, 5.188692, -0.153982, 1.251954\H, 0, 5.908927, -1.661452, 0.641599\C, 0, 2.207973, 0.81159, 2.393449\C, 0, 3.234827, 1.582668, 0.240358\C, 0, 3.975649, 2.657319, 0.785213\C, 0, 3.124746, 1.490754, -1.165843\C, 0, 4.56414, 3.618367, -0.044416\H, 0, 4.110712, 2.726428, 1.868184\C, 0, 3.726407, 2.448409, -1.994765\H, 0, 2.536175, 0.687702, -1.613224\C, 0, 4.445577, 3.517127, -1.440186\H, 0, 5.132178, 4.440687, 0.400175\H, 0, 3.624533, 2.358683, -3.080056\H, 0, 4.915877, 4.262, -2.088191\H, 0, 1.754063, 0.040056, 3.014811\H, 0, 2.275981, 1.814025, 2.8223\\Version=ES64L-G09RevD.01\State=1-A\HF=-2318.7244253\RM SD=1.035e-09\Dipole=3.514731, 0.8893513, 1.4379595\Quadrupole=4.1863384, -8.0647346, 3.8783962, 4.5985072, 5.0927251, -3.7015667\PG=C01 [X(C21H27N1O11Rh2S1)]\@

Bn-1P2

1\1\GINB-A737\SP\RBPW91\6-311++G(d,p)\C13H15N1O3S1\SI0C001\11-Apr-2018\0\#p scrf=(iefpcm, solvent=dichloromethane, smd) bpw91/6-311++G(d,p)\Title Card Required\0, 1\C, 0, 0.371418, 1.615144, 1.715441\C, 0, -1.315571, 2.646512, 0.132149\C, 0, -0.801972, 1.320297, 0.755265\C, 0, -0.380098, 0.392429, -0.402998\N, 0, -1.066244, -0.584554, -0.912681\S, 0, -2.595422, -1.022083, -0.268661\O, 0, -3.031625, 0.268267, 0.705943\C, 0, -1.929022, 0.653017, 1.568529\O, 0, -3.566646, -1.006111, -1.362054\O, 0, -2.369783, -2.215393, 0.563015\C, 0, 0.946516, 0.632054, -1.083391\H, 0, -2.363784, 1.361342, 2.289889\H, 0, -1.562129, -0.230576, 2.120021\H, 0, -1.588008, 3.347066, 0.939555\H, 0, -0.535966, 3.122009, -0.481995\H, 0, -2.206045, 2.475209, -0.490804\H, 0, 0.79026, 0.695736, 2.152553\H, 0, 1.184777, 2.149372, 1.203135\H, 0, 0.012739, 2.256709, 2.538084\C, 0, 0.981271, 1.359488, -2.220811\C, 0, 2.153764, 0.003547, -0.478571\C, 0, 3.410243, 0.64802, -0.535588\C, 0, 2.071606, -1.262147, 0.144629\C, 0, 4.551267, 0.0383, -0.002243\H, 0, 3.483629, 1.643017, -0.98342\C, 0, 3.216706, -1.86871, 0.678156\H, 0, 1.113627, -1.78671, 0.181028\C, 0, 4.459438, -1.223024, 0.607131\H, 0, 5.514087, 0.554722, -0.05287\H, 0, 3.135354, -2.853867, 1.145827\H, 0, 5.350987, -1.696594, 1.027291\H, 0, 0.076391, 1.789678, -2.655359\H, 0, 1.915561, 1.51443, -2.767021\\Version=ES64L-G09RevD.01\State=1-A\HF=-1183.0978702\RM SD=8.419e-09\Dipole=2.5850521, 2.5671037, 1.3482192\Quadrupole=-5.9166782, 3.0921501, 2.8245281, -7.893032, -5.2462285, -2.8552802\PG=C01 [X(C13H15N1O3S1)]\@

Bn-1TS6

1\1\GINB-A751\SP\RBPW91\GenECP\C21H27N1O11Rh2S1\SI0C001\24-Apr-2018\0\#p genecp scrf=(iefpcm, solvent=dichloromethane, smd) bpw91\Title Card Required\0, 1\O, 0, -3.174398, -1.312734, -1.54473\C, 0, -2.68857, -0.311743

, -2.187621\O, 0, -1.692808, 0.413301, -1.82397\O, 0, -1.003697, -3.021331, -0.771768\C, 0, 0.077442, -2.5083, -1.233608\O, 0, 0.480714, -1.29639, -1.067315\O, 0, -1.422971, -2.226731, 2.042936\C, 0, -0.454305, -1.495395, 2.44237\O, 0, 0.089093, -0.521012, 1.79296\O, 0, -3.590057, -0.52953, 1.201193\C, 0, -3.197963, 0.680002, 1.390228\O, 0, -2.074165, 1.184001, 1.028164\C, 0, -3.359368, 0.075605, -3.488632\C, 0, -4.162149, 1.616883, 2.090571\C, 0, 0.957182, -3.403181, -2.084306\C, 0, 0.087424, -1.779278, 3.831897\H, 0, 0.75428, -3.196, -3.148422\H, 0, 2.019092, -3.189819, -1.898859\H, 0, 0.735848, -4.460484, -1.885642\H, 0, 1.159367, -1.543033, 3.896724\H, 0, -0.441796, -1.141542, 4.559922\H, 0, -0.089646, -2.828646, 4.104489\H, 0, -3.997214, 0.957968, -3.315178\H, 0, -2.602254, 0.356521, -4.23479\H, 0, -3.982557, -0.748399, -3.86092\H, 0, -4.979625, 1.05168, 2.557331\H, 0, -3.630179, 2.213838, 2.846194\H, 0, -4.58242, 2.31857, 1.351634\Rh, 0, -2.311528, -1.803092, 0.238295\C, 0, 1.089432, 4.345791, 0.677945\H, 0, 1.404702, 5.362349, 0.958761\H, 0, 0.1364, 4.119616, 1.187879\O, 0, 0.898686, 4.373663, -0.754011\S, 0, -0.036731, 3.06842, -1.264615\N, 0, 0.563467, 1.793178, -0.261517\Rh, 0, -0.747357, 0.02151, -0.047777\C, 0, 1.774865, 1.988414, 0.326617\C, 0, 2.181447, 3.313519, 1.010038\C, 0, 3.553202, 3.81846, 0.512761\C, 0, 2.205583, 3.077563, 2.540635\H, 0, 3.84031, 4.732422, 1.060039\H, 0, 3.514566, 4.051116, -0.561978\H, 0, 3.015815, 2.385516, 2.82816\H, 0, 1.251209, 2.659307, 2.898423\O, 0, 0.375308, 2.859342, -2.657535\O, 0, -1.437496, 3.332858, -0.913964\C, 0, 2.693926, 0.959061, 0.197573\C, 0, 2.915807, -0.345233, 0.6487\H, 0, 2.390241, 4.028917, 3.068353\H, 0, 4.338833, 3.063031, 0.670361\H, 0, 2.15299, -0.812003, 1.297315\C, 0, 3.991755, -1.23501, 0.131115\C, 0, 4.815912, -0.849207, -0.946759\C, 0, 4.183397, -2.493741, 0.736905\C, 0, 5.819432, -1.709636, -1.403174\H, 0, 4.648737, 0.122711, -1.418901\C, 0, 5.187471, -3.354886, 0.275319\H, 0, 3.540351, -2.797237, 1.56899\C, 0, 6.00828, -2.962323, -0.79321\H, 0, 6.451924, -1.408981, -2.2428\H, 0, 5.32825, -4.330437, 0.748154\H, 0, 6.791348, -3.633931, -1.155913\H, 0, 3.457792, 0.583495, 1.303971\\Version=ES64L-G09RevD.01\State=1-A\HF=-2318.6462724\RMSD=8.993e-09\Dipole=4.2310619, -1.0613217, 3.2056222\Quadrupole=12.1976129, -10.0291868, -2.1684261, -10.5335278, 6.7420743, 17.9755554\PG=C01 [X(C21H27N1O11Rh2S1)]\@

Bn-¹TS7

1\1\GINB-A753\SP\RBPW91\GenECP\C21H27N1O11Rh2S1\SI0C001\10-May-2018\0\ \#p scrf=(iefpcm,solvent=dichloromethane,smd) genecp bpw91\\Title Card Required\\0,1\O, 0, -3.912485, 0.224558, -0.67585\C, 0, -3.268802, 1.237639, -1.135242\O, 0, -2.002295, 1.429932, -1.056348\O, 0, -2.544507, -2.170962, -1.506883\C, 0, -1.559383, -1.793008, -2.23549\O, 0, -0.664017, -0.925547, -1.917625\O, 0, -1.719434, -2.639809, 1.257178\C, 0, -0.459606, -2.454631, 1.378685\O, 0, 0.218584, -1.46165, 0.91219\O, 0, -3.110024, -0.234068, 2.050064\C, 0, -2.220991, 0.624457, 2.401896\O, 0, -1.157056, 0.928335, 1.750824\C, 0, -4.069293, 2.327637, -1.815018\C, 0, -2.454423, 1.3722, 3.69884\C, 0, -1.450452, -2.406404, -3.617749\C, 0, 0.31471, -3.500386, 2.160711\H, 0, -1.89164, -1.712548, -4.352614\H, 0, -0.39735, -2.558843, -3.894017\H, 0, -1.999927, -3.356423, -3.659899\H, 0, -0.326127, -4.362903, 2.384965\H, 0, 1.197006, -3.82999, 1.590686\H,

0,0.672327,-3.061701,3.106769\H,0,-5.062898,1.955642,-2.098431\H,0,-4.18686,3.173276,-1.117579\H,0,-3.527222,2.69937,-2.696199\H,0,-2.787058,2.39723,3.466737\H,0,-3.2253,0.871387,4.299323\H,0,-1.516175,1.449898,4.267584\Rh,0,-2.836419,-1.221498,0.284617\C,0,2.517233,3.247517,0.998409\H,0,3.250154,3.988192,1.352894\H,0,1.681776,3.211094,1.719056\O,0,2.04825,3.73669,-0.277676\S,0,0.591543,2.994709,-0.667176\N,0,0.924632,1.364633,-0.251948\Rh,0,-0.818036,0.061493,-0.094911\C,0,2.24516,1.011913,-0.083169\C,0,3.182011,1.868645,0.806442\C,0,4.56836,2.071563,0.15743\C,0,3.319425,1.228559,2.211779\H,0,5.203577,2.685442,0.819195\H,0,4.471478,2.592161,-0.80795\H,0,3.93677,0.319106,2.17792\H,0,2.331996,0.970462,2.62684\O,0,0.49017,3.150929,-2.124547\O,0,-0.4508,3.529555,0.222177\C,0,2.714647,-0.073722,-0.804621\C,0,3.818069,-1.122024,-0.623937\C,0,2.251698,-1.257349,-1.416649\C,0,4.952462,-1.212465,-1.513843\C,0,3.885876,-1.832725,0.624922\C,0,6.075604,-1.936528,-1.149414\H,0,4.908294,-0.686618,-2.471547\C,0,5.043553,-2.524125,0.988976\H,0,3.008971,-1.806704,1.275131\C,0,6.136605,-2.585676,0.108666\H,0,6.929869,-1.991084,-1.829682\H,0,5.087454,-3.041233,1.951502\H,0,7.034284,-3.142904,0.388507\H,0,3.808067,1.940005,2.901286\H,0,5.089747,1.118678,-0.011811\H,0,2.52287,-1.50213,-2.447801\H,0,1.473415,-1.876646,-0.956938\\
Version=ES64L-G09RevD.01\State=1-A\HF=-2318.6532163\RMSD=3.075e-09\Dipole=5.1464652,-3.7410494,1.153292\Quadrupole=22.5744058,-21.2318248,-1.342581,-22.7517768,5.0057672,12.3218323\PG=C01 [X(C21H27N1O11Rh2S1)]\
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[1] Zhang, X.; Xu, H.; Zhao, C. *J. Org. Chem.* **2014**, *79*, 9799.